ABAQUS/XFEM to study the fracture of 3D printed polymers considering layer interfaces

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Abstract: Additive manufacturing (or 3D printing) is being increasingly used in a wide range of areas including civil, aerospace and biomedical engineering where it offers significant advantages over conventional methods for model prototyping. However, the reduced fracture resistance typically observed in 3D printed materials limits its application to functional components. The fracture of 3D printed polymer materials with various layer orientations is studied using the extended finite element method (XFEM) with the aid of finite element software ABAQUS. Single edge notch bend (SENB) specimens made of acrylonitrile-butadiene-styrene (ABS) materials through fused deposition modeling (FDM) with various crack tip/layer orientations subjected to 3-point bending are considered. The XFEM with cohesive segment approach is employed to model the inter-laminar fracture (fracture between layers), cross-laminar fracture (fracture through layers), as well as mixed cross-/inter-laminar fracture of 3D printed ABS specimens. Both elastic and elastic-plastic fracture models are developed for the inter-laminar and cross-laminar fracture, respectively. For mixed cross-/inter laminar fracture, an anisotropic damage model is developed to predict the kinked crack propagation patterns as well as the dependence of fracture toughness on crack tip/layer orientations observed experimentally. Two damage initiation criteria were defined considering both the weak interfaces between layers and the maximum principle stress in the determination of the alternate crack growth paths. The anisotropic damage model developed in ABAQUS/XFEM through user-defined damage initiation subroutine is able to capture the fracture behavior of 3D printed polymer materials considering various layer orientations.

Keywords: 3D printing; Crack Propagation; Acrylonitrile-Butadiene-styrene (ABS); XFEM; Cohesive segment approach; Anisotropic Damage; SENB specimen

I. Introduction

The additive manufacturing (AM) process – that incorporates 3D printing – is a general term encompassing a variety of systems used to create three-dimensional physical parts and models directly from digital data. These systems are primarily manufactured using a layer by layer. Additive technologies are based on the solid modeling portion of computer-aided design. Additive systems use this solid modeling data to build in extremely thin cross-sectional layers. This permits manufacturing of intricate shapes and surfaces much more simply than by conventional methods.
Pieces can also be built from three-dimensional imaging data generated by 3D scanning or medical imaging devices. Materials used in AM are broadly classified as either liquid, powder, filament or sheets. Polymers are the primary type of materials used in AM.

Fused Deposition Modeling (FDM) is a popular layer AM technique that uses production-grade thermoplastic materials to produce both prototype and end-use parts. In which a 3D printing element is fabricated by the deposition of polymer material layer by layer. Since FDM parts are constructed with production-grade thermoplastics including ABS and Polycarbonate, they are both functional and durable. Fracture is an important mode of failure in 3D printing polymers. It governs the ultimate strength of ABS material in a variety of situations where discontinuities lead to the concentration of critical elastic-plastic strain energy release rate. Moreover, fracture is commonly distinguished between brittle and ductile mechanisms involving localized yielding and growth of micro-voids. At the material scale, fractures initiate in a ductile mode (cross-laminar crack growths) and transition into a brittle mode (inter-laminar crack growths) during crack propagation (Ghandriz, 2011). There is the interaction of behavior in the mixed cross-/inter-laminar fracture for 3D printing material.

For modeling the fracture behavior in 3D printing material, the Extended Finite Element Method (XFEM) is the most practical technique. The reason is, in the Finite Element Method (FEM), remeshing is needed whenever the model encounters discontinuity. An XFEM is a numerical method, which tries to cheat the system and allows mesh manipulation and adjusting the approximate space by incorporating enriched nodes across the discontinuity. So that is no need for mesh refinement.

The Cohesive Zone Models (CZM) were generally developed particularly for the case of modeling fracture. In the case of a certain fracture when the fracture is happened within the area of the structural dimensions, then the fracture occurs by means of material separation at certain locations. These material separation laws are defined by means of Traction- Separation Laws (TSL) in most cases. The CZM links the cohesive traction and the relative displacement across cohesive surfaces. As reviewed in Park and Paulino (2013), several cohesive constitutive relationships have been proposed in the last several decades. The corresponding mode I traction-separation relations are summarized in three groups: Traction Separation Law (TSL) with linear softening behavior, exponential softening behavior, and user defined softening behavior (Trapezoidal shaped TSL).

In this paper the vertical, horizontal and oblique laminar models were considered separately in regards to various layer orientations. The 2D plane strain anisotropic damage model with XFEM considering elastic-plastic fracture was developed by the commercial software package ABAQUS user defined subroutine. This code is able to capture the fracture performance of 3D printed polymer materials considering various layer orientation. The CZM with linear softening is employed for brittle behavior, and the exponential softening CZM has been used for ductile behavior. Also, some parameter studies were conducted using the exponential softening cohesive model for ductile fracture behavior. At the end, comparison between our computational results with the experimental ones (Kevin, 2017) was illustrated.

2. Computational Model

- Single edge notch bend (SENB) testing
Three point SENB specimen dimensioning 100×20×10 mm was assumed. Testing was performed in displacement-loading control. A 10 mm pre-crack was inserted to the mid-bottom long edge. The beam span length was 80 mm. Pins in contact with the specimen measured 6.35 mm in diameter. The applying displacement load on the mid-up long edge starts from 0.75 to 2.5 mm. Figure1 shows the assuming Three Point Bending test model.

![3PBT Model](image)

**SENB 3D Printed Material Model**

Three different laminae orientation SENB fracture specimens with consideration of crack propagation direction are depicted in Figure2: 1.) Vertically (inter-laminar fracture testing); 2.) Horizontally (cross-laminar fracture testing); and 3.) Obliquely printed (kinked laminar fracture testing), where \( \theta \) shows Crack tip/ Laminae Orientation Angle from the Y direction.

In the Abaqus computational model the first two laminar models were considered due to their specific Fracture Energy and Maximum Principal Stress (MaxPS) data, which were computed during the experimental test. The oblique laminar model, a combination of the first two laminar models' mechanical properties, considered. The XFEM, as well as the CZM, were implemented by user subroutines in ABAQUS. Table 1 shows the required mechanical properties data, which have been achieved from the ABS-M30 data sheet (ABS-M30 Sheet, 2013). Table 2 displays the value of fracture energy regarding inter-laminar and cross-laminar experiment tests (Kevin, 2017).
Figure 2. Illustration of three different SENB layer orientation.

Table 1. The ABS Mechanical properties according to two different fracture behavior.

<table>
<thead>
<tr>
<th>Mechanical Properties of ABS Material</th>
<th>Ductile Behavior</th>
<th>Brittle Behavior</th>
</tr>
</thead>
<tbody>
<tr>
<td>XZ Axis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tensile Strength, Yield</td>
<td>31 MPa</td>
<td>26 MPa</td>
</tr>
<tr>
<td>Tensile Strength, Ultimate</td>
<td>32 MPa</td>
<td>28 MPa</td>
</tr>
<tr>
<td>Tensile Modulus</td>
<td>2230 MPa</td>
<td>2180 MPa</td>
</tr>
<tr>
<td>Tensile Elongation at break</td>
<td>7 %</td>
<td>2 %</td>
</tr>
<tr>
<td>Tensile Elongation at Yield</td>
<td>2 %</td>
<td>1 %</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>0.35</td>
<td>0.35</td>
</tr>
</tbody>
</table>

Table 2. The experimental Fracture Energy result.

<table>
<thead>
<tr>
<th>Fracture Behavior</th>
<th>Critical elastic-plastic strain energy release rate (Fracture Energy) $f_{fr}$ (J/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brittle Behavior</td>
<td>256 ± 84</td>
</tr>
<tr>
<td>Ductile Behavior</td>
<td>2260</td>
</tr>
<tr>
<td>Kinked Behavior</td>
<td>256 &gt; &amp; &lt; 2260</td>
</tr>
</tbody>
</table>
**Cohesive Zone Model**

Unlike the inter-laminar fracture test, when the crack propagation illustrates brittle behavior, the crack propagation in the cross-laminar fracture test was ductile in nature and needed more energy to debond the perpendicular layers to move forward. According to the Traction-Separation relation Law model (TSL), which characterizes the material failure, the Linear softening model was considered for Brittle behavior and the Exponential softening model was applied to consider the relevant maximum cohesive strength $T_0$ and failure displacement $\delta_0$ value. The Exponential softening model results depend on the experimental law parameter ($\alpha$). If applying larger values to this parameter shows higher exponential curvature, then the computational results are more fitted to this experimental result.

Shown in Equation 1, the two independent cohesive parameters are: the Maximum cohesive strength $T_0$, which is the peak stress, and the cohesive energy $\Gamma_0$, which is the area enclosed by the TSL. The parameter $\delta$ represents the separation of the cohesive element, where $\delta_0$ is the critical displacement at failure and $\delta_{\text{init}}$ is the displacement when void initiation occurs. The stress on the cohesive element increases with the slope of cohesive stiffness $K_{\text{nm}}$, which denotes the elastic behavior until the stress reaches a critical point ($T_0$). Then, damage evolution occurs until the cohesive element loses its stress carrying ability, when the separation is equal to $\delta_0$. Figure 3 describes the parameters, and the variation of ductile model exponential softening behavior to the Exponential Law Parameter $\alpha$. Four cohesive zone models have been obtained for $\alpha$. $\alpha = 0$ expresses linear softening TSL and $\alpha = 1, 3, 10$ demonstrates the exponential softening TSL model.

$$T = \begin{cases} 
T_0 \frac{\delta}{\delta_{\text{init}}} & \text{if } \delta < \delta_{\text{init}} \\
T_0 \left(\frac{\delta_0 - \delta}{\delta_0 - \delta_{\text{init}}}\right) & \text{if } \delta_{\text{init}} \leq \delta \leq \delta_0 \\
0 & \text{if } \delta > \delta_0 
\end{cases} \quad \text{(Equation.1)}$$

The characteristic length is given by: $\delta_0 = 2\Gamma_0 / T_0$. The four traction–separation curves are shown in Figure. 4, where they are based on the two TSL models (standard bi-liner one and exponential one), and have the same Work-of-separation $\Gamma_0$ and maximum traction $T_0$. 
Figure 3. Schematic of the bi-linear and exponential Traction–Separation Law in the cohesive zone model with a varying Exponential law parameter $\alpha$.

- **Model Implementation in ABAQUS/XFEM**

  The Finite Element Model is implemented in the ABAQUS software using its XFEM capabilities. The Maximum cohesive strength $T_0$ defines the MaxPS which is assumed as a damage initiation criterion, and the cohesive energy $\Gamma_0$, is used as a fracture energy and represents the damage evolution criterion.

  In both Ductile fracture behavior (Horizontally printed layers) and Brittle fracture behavior (Vertically printed layers), the crack propagates in only one specific direction; therefore, the isotropic cohesive zone damage model was assumed. On the other hand, for the Kinked fracture behavior (obliquely printed layers), the anisotropic cohesive zone damage failure criterion model was developed to consider the mixture of crack path in two direction by the ABAQUS user subroutine, because it incorporated the weak plane failure criterion and the Maximum Principle stress criterion. In the context of kinked crack propagation criterion, the parts of the crack path between the layers were assumed by weak plane failure criterion (as shown in Equation 2), with consideration to the ABS brittle behavior properties. Also, the MaxPS failure criterion, which refers to those parts that happened across the layers, with respect to the ABS ductile behavior properties (is shown in Equation 3). The ABS brittle and ductile behavior properties are discussed in Table 1.
Weak plane failure criterion: 
\[ \left( \frac{\sigma_{11}}{\sigma_{a1-x}} \right)^2 + \left( \frac{\sigma_{12}}{\sigma_{a1-y}} \right)^2 + \left( \frac{\sigma_{13}}{\tau} \right)^2 = 1 \] (Equation 2)

Max principle stress failure criterion: 
\[ \frac{\sigma_p}{N_p} = 1 \] (Equation 3)

In Equation 2, \( \sigma_{a1-x} \) represents the axial stress occurring in the x-direction of the weak plain, \( \sigma_{a1-y} \) depicts the axial stress happening in the y-direction of the weak plain, and \( \tau \) describes the shear strength in the weak plane. In Equation 3, \( \sigma_p \) is representative of the max principal stress and \( N_p \) is a normal stress (Feerick, 2013).

CZM parameter values are selected based on the suggestions of a prior experiment (Alfano, 2015). To achieve a better match between the experiment and simulation in the Load-Displacement curve, the calibration on the initial guess of the two main CZM parameters directly from experiments (\( T_0 \) and \( \Gamma_0 \)) had been applied. In regards to various calibrations that have been noted in different literatures (Chen, 2013), calibration of the two main CZM parameters (\( \Gamma_0 \) and \( T_0 \)) in this study were made. This calibration have been applied only to the brittle behavior result as it was not fitted to the Experimental result properly. Ductile behavior agreed well with the relevant experimental result. Table 3 shows the applied calibration.

<table>
<thead>
<tr>
<th>The CZM parameters</th>
<th>Before Calibration</th>
<th>After Calibration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cohesive Energy ( \Gamma_0 ) =fracture energy ( (J_{IC}) )</td>
<td>256 ± 84 (J/m²)</td>
<td>700 (J/m²)</td>
</tr>
<tr>
<td>Cohesive Strength ( T_0 ) =yield stress ( (\sigma_y) )</td>
<td>26 MPa</td>
<td>24 MPa</td>
</tr>
</tbody>
</table>

3. Results and Discussion

Figure 4 illustrates the simulation crack propagation in three stages, from (a) brittle, to (b) ductile, to (c) kinked fracture behavior. The crack propagates upwards in a straight line from its original position (pre-crack) sharply between the layers (\( \theta = 0^\circ \)) toward the applying displacement area. The Maximum Principal Stress (MaxPS) contour illustrates this behavior as well (Figure 4 a). Notably, more stress was required to initiate cross-laminar fracture (\( \theta = 90^\circ \)) and for the crack to propagate upwards in a straight line through the layers (Figure 4 b). The Stress countour in Figure 4 (c) shows the kinked crack path in the oblique lamina/crack-tip orientations ( \( \theta = 75^\circ \)), which combines the path between the layer and across the layers.
In Figure 5 (a), (b), and (c), are the baseline comparison curves between experimental and simulation results, in regards to the load-displacement curve as indicated. The simulation in Figure 5(a) depicts the Linear-elastic loading behavior. The results illustrate a sharp drop in the curve for brittle behavior. The results in Figure 5(b) represents the ductile Non-linear elastic-plastic loading behavior with a gradual decrease in the curve. The simulation results provide a load vs. displacement curve for a sample with $\theta = 75^\circ$ in Figure 5(c). Initially, linear-elastic loading behavior, along with non-linear elastic-plastic, represented the inter-laminar crack path brittle behavior, which succeeded the cross-laminar ductile behavior.

Figure 6, illustrates the load-displacement curve by means of comparing the energy release rate for the three distinct fracture behaviors. The area under the load-displacement curve represents the energy that was spent to form the crack propagation until the failure. As shown in Figure 6, the energy release rate was used in an oblique test is higher than a vertically printed test and lower than a horizontally printed test, for approximately the same crack propagation length.

In addition, low energy was required to debond the vertically printed layers($\theta = 0^\circ$). Notably, more energy was required to initiate cross-laminar fracture ($\theta = 90^\circ$) and propagate the crack through the layers. Separating the horizontal layers required more energy for crack propagation than the vertical layers.
Figure 5 (a). Simulation and Experimental result of Load VS. Displacement curve for vertically printed layered SENB.

Figure 5 (b). Simulation and Experimental result of Load VS. Displacement curve for horizontally printed layered SENB
Figure 5 (c). Simulation and Experimental result of Load VS. Displacement curve for oblique printed layered SENB

Figure 6. Comparison of three different fracture behaviors in one frame.
4. Conclusion

This study confirms the ability of ABAQUS/XFEM to analyze 3D printed layered material. It can accurately model the behavior of interfaces between 3D printing layers. The XFEM technique permits the application of two damage criteria, which provides the ability to change the fracture behavior in one material with different 3D printing directions: vertically, horizontally and obliquely printed layers. Moreover, Comparison of three fracture behavior Load-Displacement curves (Figure 6) illustrates the maximum peak-load happens in the Ductile fracture behavior (Cross-Laminar SENB). However, the peak-load in the brittle behavior (Inter-Laminar SENB) is considerably less than the other two fracture behaviors. To clarify off axis crack prediction in kinked fracture of AM polymers, crack path direction is determined perpendicularly to the defined MaxPS direction. The oblique crack-tip/laminae orientation illustrates the kinked crack path that follows the weak inter-laminar plane in response to the maximum principal stress cross-laminar plane. It means the XFEM is particularly suitable for modelling crack propagation phenomena, without knowing the crack path beforehand.

5. References


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