Additive Manufacturing

- Lightweight
- Favorable mechanical properties
- Multifunctional application
- Add details to design with low manufacturing costs
- High process speed
- Build a large range of prototypes with complex geometries

Background


Aerospace trim tool being printed at ORNL’s BAAM system - 5.2 m long structure made of ABS with 20% carbon fiber [1].
Background

Acrylonitrile butadiene styrene (ABS)
- High rigidity
- Good impact resistance, even at low temperatures
- Good insulating properties
- Good abrasion and strain resistance
- High dimensional stability (Mechanically strong and stable over time)
- High surface brightness and excellent surface aspect


Background

Carbon Fiber Reinforced composites
- Advantages of Carbon Fiber (CF) filled polymers in FDM
  - High strength to weight ratio
  - Excellent fatigue, corrosion and wear resistance
  - Higher modulus (up 4.5X with 13% CF/ABS [4])
  - Higher strength (up 3X with 13% CF/ABS [4])
  - Increased thermal conductivity
  - Improved dimensional stability
- Significant advantage of CF in FDM materials:
  - Improved directional properties in bead
  - Ability to print in preferred direction
- Bead Microstructure Properties
  - Fibre Volume fraction
  - Fibre Orientation
  - Voids

Background

Fiber Orientation Tensor

Fiber orientation is calculated using orientation tensors \cite{Advani1987}:

\[
\frac{DA}{dt} = -\frac{1}{2}(\Omega \cdot A - A \cdot \Omega) + \frac{1}{2} \lambda(\Gamma \cdot A + A \cdot \Gamma - 2A \circ \Gamma) + D_r,
\]

Where:

\[
A_{ij} = \oint p_i p_j \psi(p) dS \quad (\text{2nd order fiber orientation tensor})
\]

\[
A_{ijkl} = \oint p_i p_j p_k p_l \psi(p) dS \quad (\text{4th order fiber orientation tensor})
\]

\[
A_{ijl}=A_{ijk}=A_{ikl}=A_{ijkl}=A_{ikjl}
\]

\[
A_{ijkk}=A_{jik}=A_{jki}=A_{ikj}=A_{kji}=A_{kij}
\]

\[
\psi = \text{the probability density function for fiber orientation}
\]

\[
D_r = \text{Rotary Diffusion Function}
\]

Background

Factors Influencing Void Formation

- Air entrapment in flow process during compounding & processing stages begins the process
- Experiment shows nucleation occurs at fiber ends
- Fluid/Flow parameters (shear rate, temperature, fiber conc.in terms of viscosity) ultimately determines void formation
- Difference in the matrix-fiber coefficient of thermal expansion leads to more porosity in the print
- Differential cooling rate between the external surface and core regions leads to more voids
- Aspect ratio also influences void content

\cite{Advani1987, Cintra1995, Vaxman1989}
Background

Void Distribution during the Fiber Reinforced Polymer Deposition Process

Most pores are formed at the die exit due to die swell.

Decrease in porosity during on-bed deposition due to escape of air bubbles before cooling.


Experimental Evaluation of Microstructure Properties

Experimental parameters:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>210 ºC</td>
</tr>
<tr>
<td>Printing Height</td>
<td>2.5 mm</td>
</tr>
<tr>
<td>Screw Speed</td>
<td>2250 RPM</td>
</tr>
<tr>
<td>Nozzle Diameter</td>
<td>3.175 mm</td>
</tr>
</tbody>
</table>

13 wt% Carbon fiber reinforced ABS 3D printed using LAAM system

Buehler IsoMet Low Speed saw

NSI X3000 micro-CT system [10].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Voltage</td>
<td>60 kV</td>
</tr>
<tr>
<td>Current</td>
<td>900 µA</td>
</tr>
<tr>
<td>Resolution</td>
<td>2.8 µm</td>
</tr>
<tr>
<td>Time</td>
<td>8.35 h</td>
</tr>
</tbody>
</table>

NSI X3000 micro-CT scan parameters
Results - Voids Distribution

- The voids size were determined by the diameter of the circumscribed sphere of the void.
- The largest void has a diameter of 1.76 mm and, the smallest one is 0.04 mm in diameter.
- The void volume ratio within this AM part is 6.26%.
- The void’s sphericity is varied between 0.01 to 0.75 within the AM part:

\[
\text{Sphericity} = \frac{A_{\text{sphere}}}{A_{\text{void}}}
\]

Results - Voids Distribution

- Voids Distribution along Different Directions

Void distribution along the width of AM part

Void distribution along the thickness of AM part

Void distribution along the printing direction of AM part
Results – Fiber Orientation

Fiber Orientation along Different Directions

- Along the width of the AM part
  - Carbon Fiber Distribution Characterized By Micro-CT
- Along the thickness of the AM part
- Along the printing direction of the AM part

Results – Fiber Volume Fraction

Fiber Volume Fraction along Different Directions

- Along the width of the AM part
- Along the thickness of the AM part
- Along the printing direction of the AM part
Simulation of Micro-Void Development within Beads

- **Objective**
  - To better understand mechanisms that promote void formation within beads produced by BAAM polymer composite deposition

- **Hypothesis**
  - Voids nucleate on low pressure regions on fiber surface during deposition process

- **Methods**
  - Multiscale Model
    - Macro-Model (2D Planar Deposition Flow Model)
      - Predicts Flow Field in Nozzle (velocity streamlines, gradients and pressure)
      - Predict Fiber Orientation Tensors
    - Micro Model
      - Single Fiber Evolution through Jeffery’s orbit
        - Simulates evolution of a single ellipsoidal fiber suspension in polymeric melt flow, Inputs are based on responses from Macro-Model
      - Jeffery’s Analytical Model (*Verification purpose only*)
        - Interface Btw Macro & Micro Model

Macro-Model - 2D Planar Deposition Flow Model

- Steady Stokes flow
- Decoupled flow simulation
  - Fiber presence ignored during flow computation

**Governing Equations**

\[ \nabla \cdot \mathbf{v} = 0 \]

\[ \nabla \cdot \mathbf{\sigma} + \rho f = 0, \]

\[ \mathbf{\sigma} = \tau - P \mathbf{I} \]

\[ \tau = 2\mu D \]

**Software**

ANSYS – Polyflow

- The polymer melts in the barrel and is forced through the nozzle and extruded onto the moving plate or pre-deposited material below

**Macro-Model- 2D Planar Deposition Flow Model**

Simulation Results – Component Velocities

**Material:** 13% carbon fiber filled ABS

<table>
<thead>
<tr>
<th>Fluid Properties @230°C</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity of Melt</td>
<td>817 [Pa s]</td>
</tr>
<tr>
<td>Density</td>
<td>1154 [kg/m³]</td>
</tr>
<tr>
<td>Shear rate</td>
<td>100 [s⁻¹]</td>
</tr>
</tbody>
</table>

Streamlines Deposition times:

\[ t_{10} = 1.112s, \quad t_{15} = 1.487s, \quad t_{18} = 2.780s \]

**Micro-Model – 2D Single Fiber Evolution Model**

**Model Assumptions**

- Steady state \( \frac{\partial}{\partial t} \rightarrow 0 \)
- Incompressible fluid \( \frac{\partial \rho}{\partial t} = 0, \quad \nabla \cdot \mathbf{u} = 0 \)
- Low Reynolds Number (Negligible Inertia) \( \nabla \cdot \mathbf{v} \approx 0 \)
- Temperature Independent fields \( \nabla T = 0 \)
- Isotropic, homogenous, Symmetric, linear - Newtonian fluids \( \tau_{ij} = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij} = 2\mu\varepsilon_{ij} \)
- No slip at fluid and fiber edge and no flux through the fiber surface

**Definitions**

\[
\begin{bmatrix}
\frac{\partial}{\partial x} \\
\frac{\partial}{\partial y} \\
\frac{\partial}{\partial z}
\end{bmatrix}
\begin{bmatrix}
\xi \\
\xi_x \\
\xi_y
\end{bmatrix} = \begin{bmatrix}
\tau_x \\
\tau_y \\
\tau_z
\end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix}
u_x \\
u_y \\
u_z
\end{bmatrix}
\]

**Usable Form**

\[
\begin{align*}
\nabla \cdot \mathbf{u} &= 0 & \text{ - Continuity} \\
\nabla \cdot \mathbf{\sigma} + \rho f &= 0, \quad \mathbf{a} = \mathbf{\tau} - \rho \mathbf{1} & \text{ - Momentum} \\
\mathbf{\tau} &= \mathbf{C}_f \nabla \mathbf{u} & \text{ - Constitutive}
\end{align*}
\]

Developed based on a custom FEA code written in MATLAB

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Sayah, Awenlimobor, Wang, and Smith - Baylor University
Micro-Model – 2D Single Fiber Evolution Model

- Transformed Galerkin Equations
  - Continuity
    \[ \int_{\Omega} \frac{\partial (\frac{\partial u}{\partial x})}{\partial t} d\Omega + \int_{\Gamma} \frac{\partial (\frac{\partial u}{\partial x})}{\partial n} d\Gamma = 0 \]
  - Momentum
    \[ \int_{\Omega} \frac{\partial (\mu e)}{\partial t} d\Omega + \int_{\Gamma} \mu \frac{\partial e}{\partial x} d\Gamma - \int_{\Omega} \rho \frac{\partial e}{\partial t} d\Omega - \int_{\Gamma} \frac{\partial e}{\partial t} d\Gamma = 0 \]

- Boundary Condition
  \[ u_1 = [u_1 u_2] = u_{BC1} \]
  \[ u_2 = [u_1 u_2] = u_{BC2} = p_0 \]
  \[ u_3 = [u_1 u_2] = u_{BC3} = u_1 + \omega \times r \]

- Element Selection

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Micro-Model – 2D Single Fiber Evolution Model

- FEA Formulations – Mixed Method
  - Mesh Consideration
  - Element Stiffness Matrix
    \[ K^e = \begin{bmatrix} \int B^T \mu B & \int B^T \phi e \frac{\partial}{\partial x} \\ \int - \phi e B & 0 \end{bmatrix} \]
  - Element Force Vector
    \[ f^e = \begin{bmatrix} \int \rho \frac{\partial e}{\partial t} d\Omega + \int \frac{\partial e}{\partial t} d\Gamma \\ 0 \end{bmatrix} \]
  - Solution Variables
    \[ \begin{bmatrix} U^e \end{bmatrix} = \begin{bmatrix} U \end{bmatrix} = \begin{bmatrix} F \end{bmatrix} = \begin{bmatrix} F^e \end{bmatrix} \]
  - Assembly Matrix & Partitioning
    \[ K U = F \]

\[ \begin{bmatrix} K_{ff} & K_{fe} \\ K_{ef} & K_{ee} \end{bmatrix} \begin{bmatrix} U_f \\ U_e \end{bmatrix} = \begin{bmatrix} F_f \\ F_e \end{bmatrix} \]

Single stage solution → \[ U_f = K_{ff}^{-1}(F_f - K_{fe}U_e) \]
\[ F_e = K_{ef}U_f + K_{ee}U_e \]

Image Source: Ref [6]

### Micro-Model – 2D Single Fiber Evolution Model

- **Computing Fiber’s Velocities**
  - Hydrodynamic Force and Torque
    \[ F_I = -\sum_{n \in N} E_{BC}^n, \quad T_I = -\sum_{n \in N} \frac{r_n \times E_{BC}^n}{\mu} \]
  - Newton Raphson Iteration
    \[ \begin{align*}
    \Delta U &= \frac{\partial U}{\partial \phi} \Delta \phi \\
    \Delta U &= \frac{\partial U}{\partial \phi} \frac{\partial \phi}{\partial \phi} = \frac{\partial U}{\partial \phi} = 0
    \end{align*} \]

- **Updating Fiber’s Position**
  - 4th Order Runge Kutta Iteration
    \[ t_{i+1} = t_i + k \Delta t, \quad \Delta x = \frac{h}{2} \frac{\partial U}{\partial x} + \frac{h}{2} \frac{\partial U}{\partial y} \]

### Assumptions
- Torque Free fiber particle
- Creeping, Incompressible, Newtonian, Simple Shear homogenous flow
- \[ U_{BC} = U_{BC} = 0, \quad U_{BC} = \gamma y \]
- Time period for tumbling motion
  \[ T = \frac{2\pi}{y} \left[ r_e + 1/r_e \right] \]
- Fiber Orientation Angles
  \[ \phi(t) = \tan^{-1} \left( \frac{\tan \theta}{1 + \tan \theta} \right) \]
  \[ \theta(t) = \tan^{-1} \left( \sqrt{\frac{r_c \cos^2 \phi + \sin^2 \phi}{\cos^2 \phi + \sin^2 \phi}} \right) \]

### Micro-Model - Jeffery’s Analytical Model

- **2D simplification**
  \[ C = +\infty \text{ such that } \theta = \pi/2, \quad \phi = 0, \quad \psi = 0 \]
  \[ \phi(t) = \tan^{-1} \left( \frac{r_c \tan \frac{\pi}{2}}{r_c + 1/r_c} \right) \quad \text{- Orientation angle} \]
  \[ \phi = \frac{r_c \tan \frac{\pi}{2}}{r_c + 1/r_c} \quad \text{- Angular velocity} \]

- **2D Model Justification**
  - Ability to reproduce Jeffery’s Orbit
  - A first step in understanding the process of voids nucleation
  - Utilize data from previous work on 2D planar deposition flow
Results – Constant B.C’s

- Model Validation - Jeffery’s Orbit

- Result Summary
  - Good agreement btw. FEA and Jeffery’s Calculation
  - Fiber experienced a drop in minimum pressure along Jeffery’s Orbit
  - Location of dip on fiber’s surface is close to the fiber’s tip/edge
  - Supports our hypothesis of potential void nucleation at these location, based on literature.

Results - Constant B.C’s

- Shear Rate Sensitivity
  - Fiber’s Spin and Spin rate increases with shear rate
  - Pressure Extremes are more severe with higher shear rate

- Aspect Ratio Sensitivity
  - Smaller aspect ratio has smaller time period
  - Minimum pressure decreases with increasing aspect ratio [3]

Results – Streamline Dependent B.C’s

- Velocity Gradient Contours

- Dominant gradient: $\frac{\partial V_y}{\partial x}$
- Shear rates are relatively lower closer to the center streamline and more severe towards the nozzle edges
- Singularities at nozzle tip where flow transitions from no-slip to a free surface BC
- Uniform velocity and zero shear rates on plate/bed
- Satisfies Continuity

$$\frac{\partial V_x}{\partial y} + \frac{\partial V_y}{\partial x} = 0$$


Results – Streamline Dependent B.C’s

- Input: Streamline Velocities
- Input: Streamline Velocity Gradients
- Output: Fiber’s Orientation Angle
- Output: Fiber’s Angular Velocity

- Relatively lower fiber spin and spin rates on streamlines towards the center compared to streamlines out towards the nozzle edge
- More severe gradients for edge streamlines responsible for higher values

$\psi_{10}$

$\psi_{18}$
Results – Streamline Dependent B.C.’s

- **Fiber’s Extreme Pressure History**

  - Minimum pressure drop on the fiber’s surface at the nozzle exit is seen to be higher for streamlines closer to the center compared to those farther towards the edge.
  - Pressure results indicates the likelihood of void formation near fibers in BAAM deposition flow.

Conclusion

- 3D printed short carbon fiber reinforced ABS bead contains a large number of voids (volume fraction 6.26%) with various size and shape.
- Voids are randomly distributed in the sample.
- Voids tend to form near the carbon fibers.
- Sphericity of voids varies over the sample.
  - Few Voids have the irregular shape (sphericity between 0.1 to 0.35).
  - Most voids are more spherical in shape (sphericity between 0.50 to 0.70).
- Carbon fiber volume fraction (7%) remains constant along the printing direction.
- Carbon fiber alignment varies through the sample.
  
  Orientation Tensor $A_{ij} = \begin{bmatrix} 0.25 & 0.02 & 0.08 \\ 0.02 & 0.16 & -0.03 \\ 0.08 & -0.03 & 0.60 \end{bmatrix}$
  
  - Fibers tend to align in the printing direction.
  - Fibers are more aligned near the edge of the bead.
  - Fibers are less aligned near the center of the bead.
Conclusion

- Multiscale approach has been developed for predicting fiber motion and fluid pressure around single fibers in polymer composite deposition flow
- Single fiber model predicts Jeffrey's orbit
- Aspect ratio is shown to influence minimum pressure on fiber surface
- Results show significant minimum pressure on the fiber surface during BAAM polymer composite deposition
- Minimum pressure is shown to be streamline dependent
- Model results indicate the likelihood of void formation near fibers in BAAM deposition flow.

Future work

- Investigate more samples to understand the variability in results
- Perform the parameters study to understand the effect of different printing parameters on carbon fiber orientation and void content, and their distribution in the bead
- Develop a model for particle migration in polymer flow
- Extend multi-scale modeling approach to 3D flow simulation
- Investigate effect of initial fiber angle and streamline location on minimum pressure prediction
- Develop a relationship between print processing parameters and likelihood of void formation
- Implement a Generalize Newtonian Fluid model in the nozzle flow and single fiber model
- Establish a relationship between minimum pressures and void initiation