SPE ACCE
September 6-8, 2023

Simulating the Effect of Bead Micro Structure on Interlayer Adhesion in Large Area Additive Manufacturing Polymer Composite Deposition

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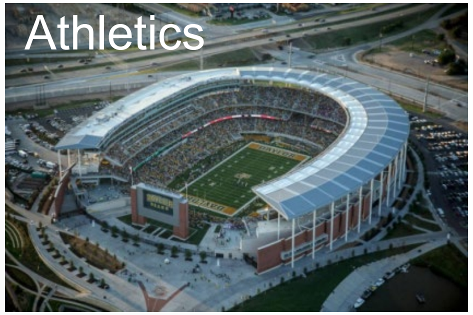
NSF Award Number 2055628

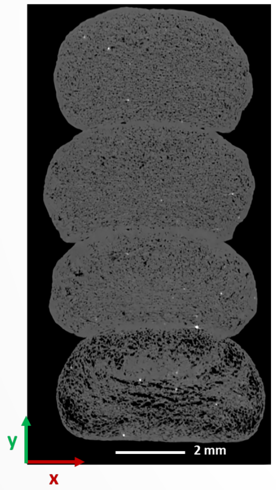


Presentation Overview

OBJECTIVE

Assess the effect of materials and processing (i.e., carbon fiber content and orientation, voids, print location) on bead adhesion in a single bead stack from Large Area Additive Manufacturing (LAAM) polymer composite deposition.

OUTLINE



Introduction

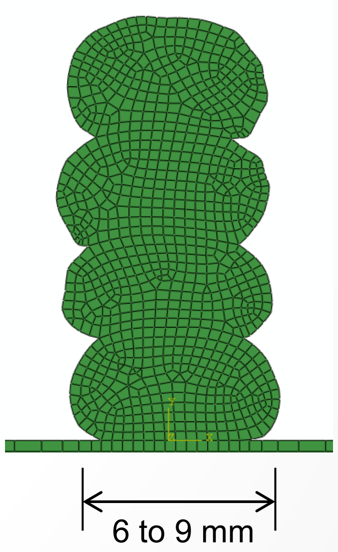
Fiber Orientation and Adhesion Analysis

LAAM Bead Preparation and Inspection

Transient Thermal FEA

Adhesion Assessment

Conclusions

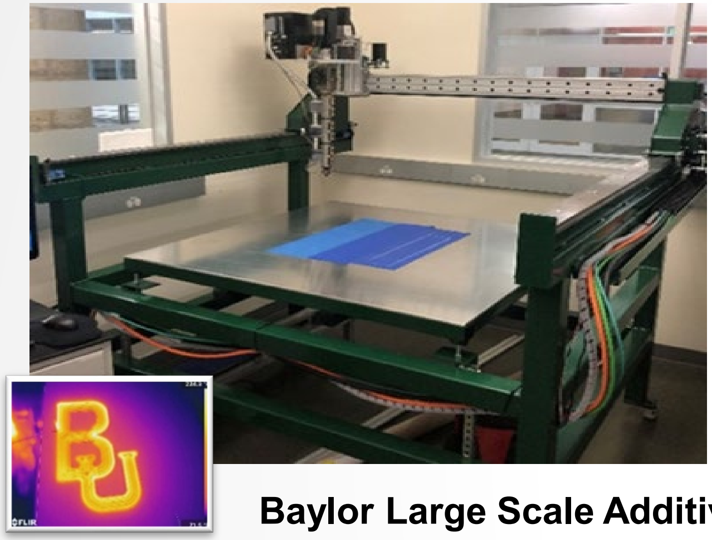


Baylor University

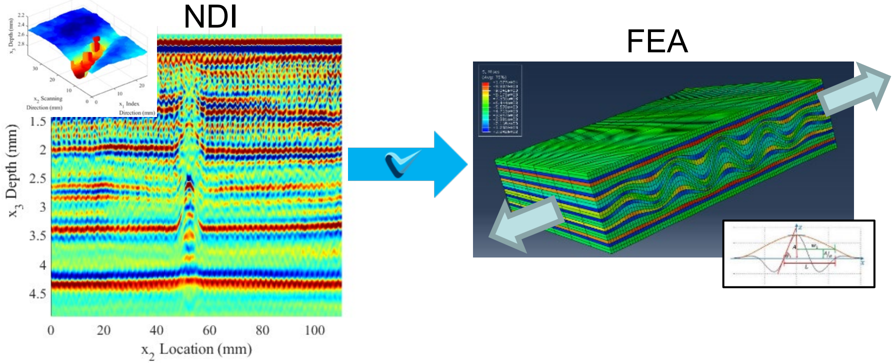
- **Baylor University was chartered in 1845 by the Republic of Texas under the mission of Pro Ecclesia and Pro Texana**
- **Baylor has an enrollment of 18,000 students (14,000 undergraduate) in 127 undergraduate, 78 master's, and 46 doctoral programs**
- **Baylor named a Research 1 University in 2021!! 1 of 137 in US, 1 of 37 private universities.**
- **In 2004 ENG offered master's degrees, and in 2006 the departments of Mechanical Engineering (ME) and Electrical and Computer Engineering (ECE) were formed.**
- **In 2014 ME began their PhD program, and ECE began theirs in 2011**
- **ME PhD Spring 2023 enrollment of 46 PhD students.**
- **Baylor Materials Lab: 6 faculty, 19 PhD students, 8 professional staff, 12K ft^2 lab/office space, funding via Verifi Tech., NSF, Sandia National Labs, L3-Harris, NASA, AFOSR, ONR, ORNL, Spirit Aero., Lemond, Axion, etc…**
- **Current job opening in our Materials Lab for Post Doc in Additive Manufacturing**

Baylor BRIC

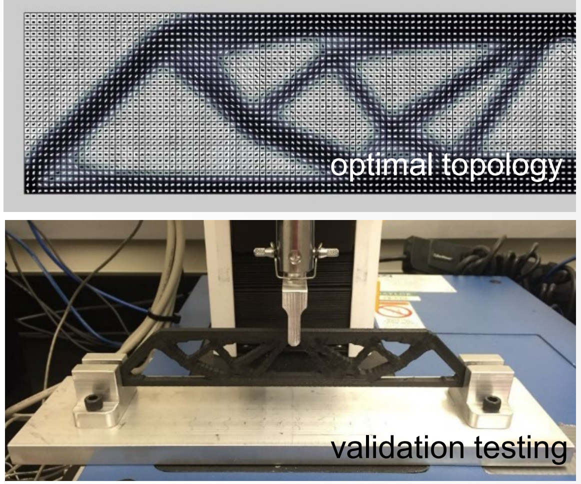
Carbon Fiber Composites AM Research



Baylor Large Scale Additive Manufacturing (LAAM)

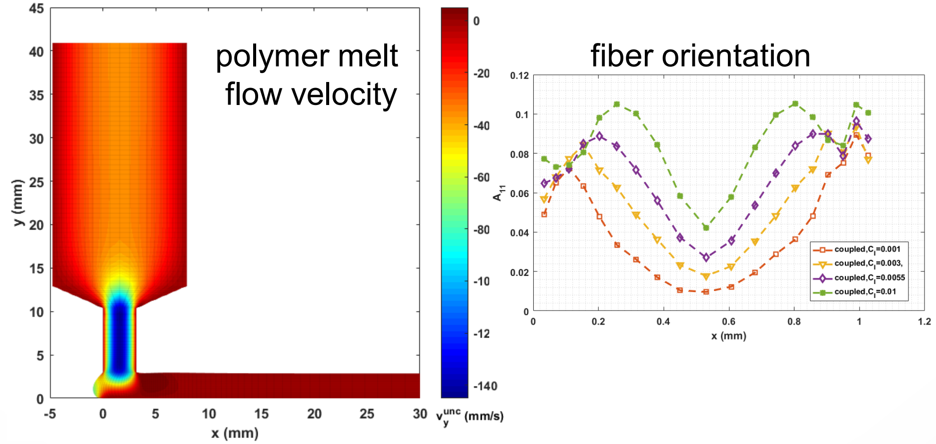


Laminated Composite NDI ➔ FEA

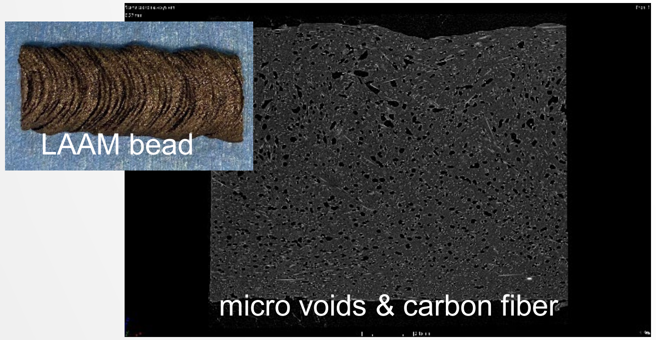


Topology Optimization for Additive Manufacturing

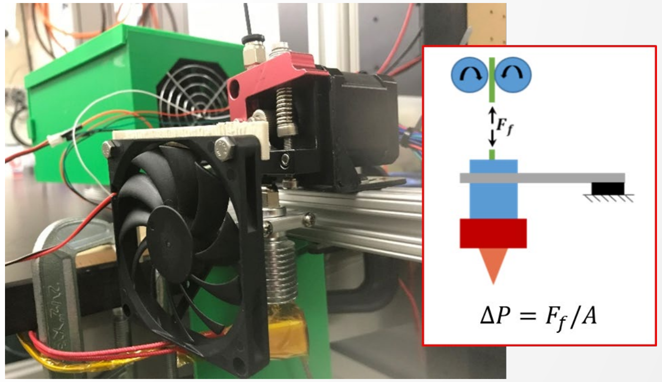
LAAM Bead Deposition Simulation



Polymer Composite Inspection for Additive Manufacturing



3D Printing Filament Rheometer



INTRODUCTION

Large Scale Additive Manufacturing

Polymer Composite Extrusion/Deposition AM


ORNL Strati – printed in 44 hrs


ORNL Shelby Cobra


ORNL 3D printed house & utility vehicle

Tooling Applications


wind turbine blade mold

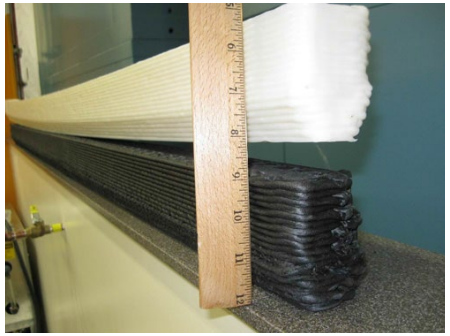

boat hull master pattern


sand casting core

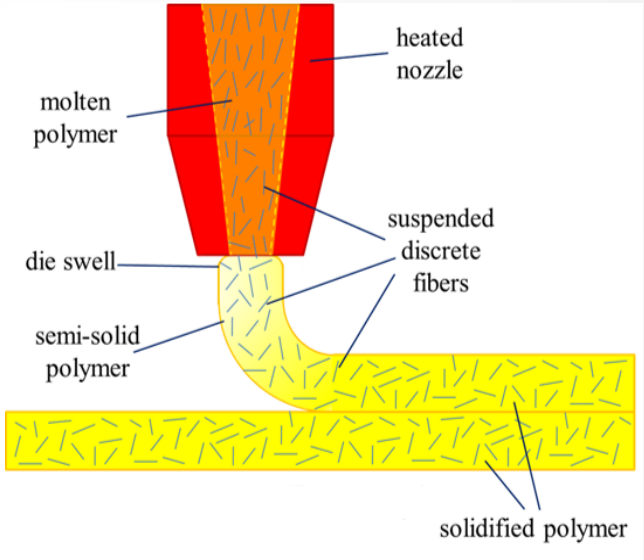

layup tooling for composites

Carbon Fiber ABS in Additive Manufacturing

- Advantages of Carbon Fiber (CF) filled polymers in FDM
  - Higher modulus (up 4.5X with 13% CF/ABS [1])
  - Higher strength (up 3X with 13% CF/ABS [1])
  - Processed with same equipment
  - Increased material selection
  - Decreased CTE
  - Increased thermal conductivity
  - Increased part dimensional stability

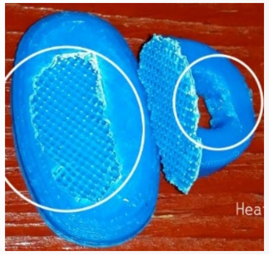


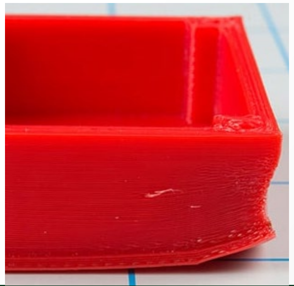
taken from Tekinalp [1]

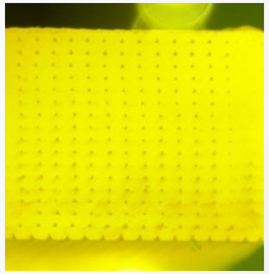


- Fibers suspended in molten polymer align with shear and extensional flow directions

- Drawbacks of polymer extrusion/deposition process:
  - Weak inter-bead adhesion
  - Inferior mechanical properties
  - Predicting printability limitted
  - Warpage
  - Voids





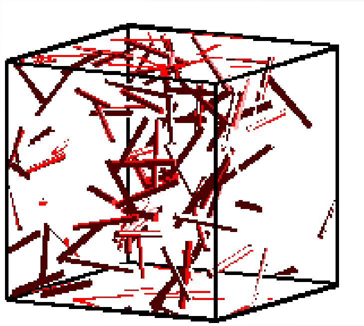


[1] H.L. Tekinalp, V. Kunc, G.M. Velez-Garcia, C.E. Duty, L.J. Love, *Comp. Sci. Tech.* 105 (2014) 144-150

FIBER ORIENTATION AND ADHESION ANALYSIS

Fiber Orientation Tensor Prediction

- **Fiber orientation is calculated using orientation tensors [1]**



$$\frac{DA}{Dt} = -\frac{1}{2}(\Omega \cdot A - A \cdot \Omega) + \frac{1}{2}\lambda(\Gamma \cdot A + A \cdot \Gamma - 2\mathbb{A}:\Gamma) + D_r$$

where:

$A_{ij} = \oint p_i p_j \psi(\mathrm{p})\mathrm{dS}$ = **the 2nd order fiber orientation tensor**

$\mathbb{A}_{ijkl} = \oint p_i p_j p_k p_l \psi(\mathrm{p})\mathrm{dS}$ = **the 4th order fiber orientation tensor**

ψ = **the probability density function for fiber orientation**

p = **the unit vector along the length of the fiber**

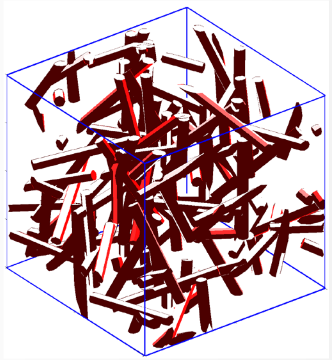
$\Omega = \left[(\nabla \mathrm{v}) - (\nabla \mathrm{v})^{\mathrm{T}}\right]$ = **the vorticity tensor**

$\Gamma = \left[(\nabla \mathrm{v}) + (\nabla \mathrm{v})^{\mathrm{T}}\right]$ = **the strain rate tensor**

D_r = **Rotary Diffusion Function**

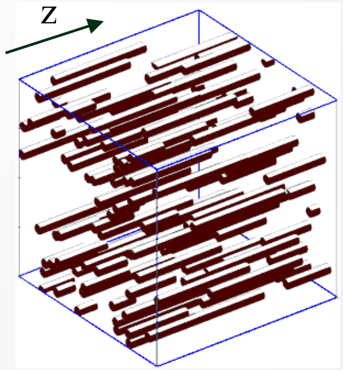
Random Orientation

$$A_{ij} = \begin{bmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \end{bmatrix}$$



Uniaxial Alignment

$$A_{ij} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



- **Fiber orientation tensor approach provides a computationally efficient means to predict fiber microstructure which is used in major mold filling software.**

Moldex3D MOLDING INNOVATION

moldflow®

[1] Advani, S., Tucker III, C., 1987. "The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites". Journal of Rheology, Vol. 31

Short Fiber Composite Properties

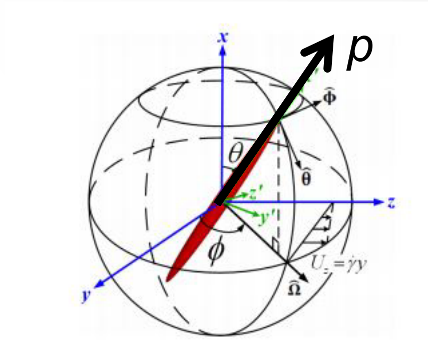
- Computing elastic properties for unidirectional short fiber composites [1]
  - Methods: Bounding model, Eshelby's equivalent inclusion, Self-constraint method, Halpin-Tsai, Mori-Tanaka, or Lielens

- For misaligned fibers, the closed form expressions of material stiffness derived in Jack and Smith 2006 [2] are used
  - Orientation homogenization method
  - Stiffness prediction is based on the fiber probability orientation distribution $\psi(\theta,\phi)$

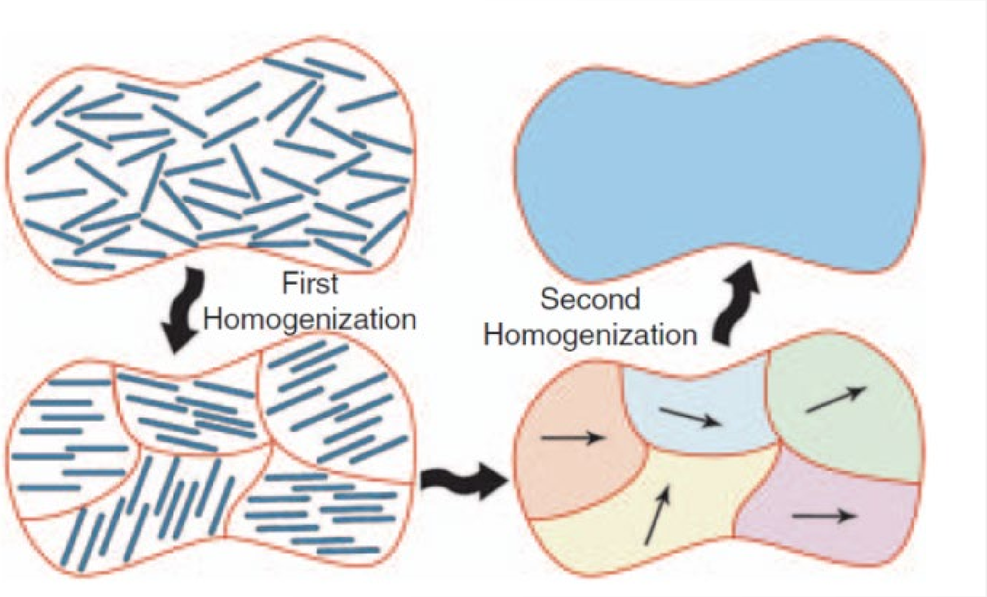
$$\langle C_{ijkl}\rangle = \oint_{\boldsymbol{S}^2} \boldsymbol{Q}_{pi}(\theta,\phi)\,\boldsymbol{Q}_{qj}(\theta,\phi)\boldsymbol{Q}_{rk}(\theta,\phi)\boldsymbol{Q}_{sl}(\theta,\phi)\bar{\boldsymbol{C}}_{pqrs}\psi(\theta,\phi)d\boldsymbol{S}$$

  - Orientation averaged conducitivity tensor evaluated in a similar manner [3]

$$\langle k_{ij}\rangle = \oint_{\boldsymbol{S}^2} \boldsymbol{Q}_{pi}(\theta,\phi)\,\boldsymbol{Q}_{qj}(\theta,\phi)\bar{k}_{pq}\psi(\theta,\phi)d\boldsymbol{S}$$



fiber direction vector



material homogenization process

[1] G.P. Tandon, G.J. Weng, The Effect of Aspect Ratio of Inclusions on the Elastic Properties of Unidirectionally Aligned Composites, Polym. Composite. 5 (4) (1984) 327-333.
[2] D.A. Jack, D.E. Smith, The Effect of Fiber Orientation Closure Approximations on Mechanical Property Predictions, Comp. A-Appl. S. 38 (3) (2006) 975-982.
[3] B. Heller, PhD Thesis, Baylor University (2019)

Orientation Averaged Thermal Conductivity

- **Given 2nd order fiber orientation tensor A_{ij} and composite constituent component values, the orientation-averaged conductivity tensor is [1]**

$$\langle k_{ij}\rangle = \begin{bmatrix} \beta_1 & A_{12}(\bar{k}_{11}-\bar{k}_{22}) & A_{13}(\bar{k}_{11}-\bar{k}_{22}) \\ A_{12}(\bar{k}_{11}-\bar{k}_{22}) & \beta_2 & A_{23}(\bar{k}_{11}-\bar{k}_{22}) \\ A_{13}(\bar{k}_{11}-\bar{k}_{22}) & A_{23}(\bar{k}_{11}-\bar{k}_{22}) & \beta_3 \end{bmatrix}$$

where

$$\beta_1 = \frac{1}{3}\left[(1+2A_{11}-A_{22}-A_{33})\bar{k}_{11} + (2-2A_{11}+A_{22}+A_{33})\bar{k}_{22}\right]$$

$$\beta_2 = \frac{1}{3}\left[-(-1+A_{11}-2A_{22}+A_{33})\bar{k}_{11} + (2+A_{11}-2A_{22}+A_{33})\bar{k}_{22}\right]$$

$$\beta_3 = \frac{1}{3}\left[-(-1+A_{11}+A_{22}-2A_{33})\bar{k}_{11} + (2+A_{11}+A_{22}-2A_{33})\bar{k}_{22}\right]$$

Constituent Components

$k_m = k_{matrix}$

$k_f = k_{fiber}$

v_f = fiber volume fraction

$^l/_d$ = fiber aspect ratio

PolyOne

parameter	value
ABS & CFABS Supplier	PolyOne Crop. Avon Lake, OH
CF weight %	13
CF vol %	8.4
mean *l/d*	43.6

- **Unidirectional thermal conductivities are computed from [2]**

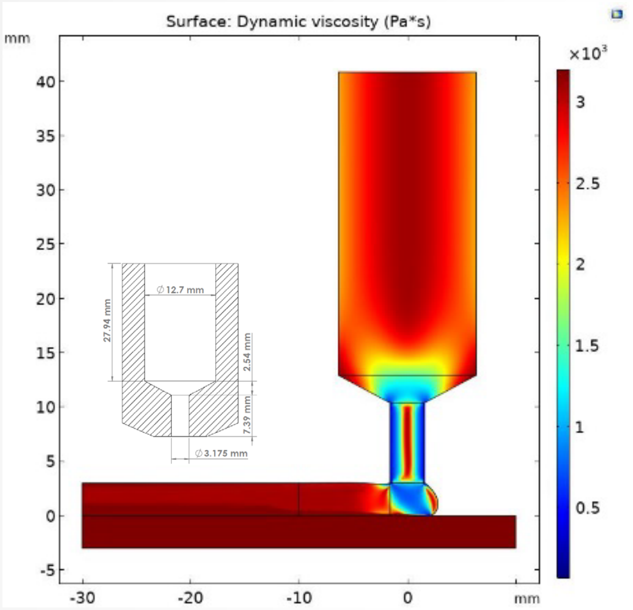
$$\bar{k}_{11} = \frac{1+2\left(^l/_d\right)\mu_1 v_f}{1-\mu_1 v_f} k_f \qquad \bar{k}_{22} = \frac{1+2\mu_2 v_f}{1-\mu_2 v_f} k_f$$

where

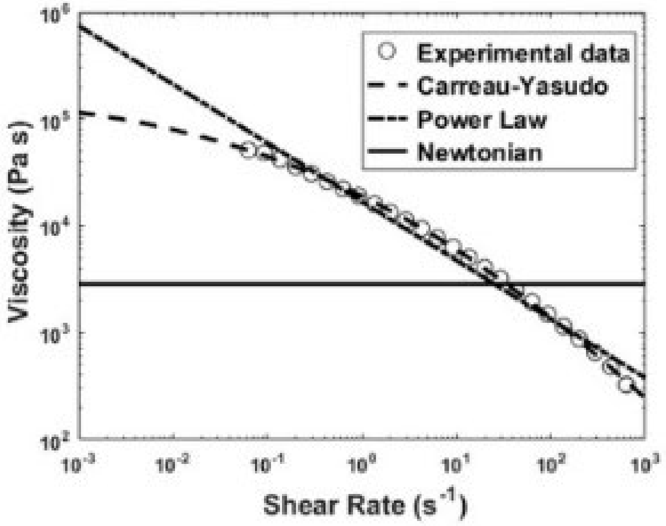
$$\mu_1 = \frac{^{k_{f1}}/_{k_m} - 1}{^{k_{f1}}/_{k_m} + 2\,^l/_d} \qquad \mu_1 = \frac{^{k_{f2}}/_{k_m} - 1}{^{k_{f2}}/_{k_m} + 2}$$

[1] B. Heller, PhD Thesis, Baylor University (2019)
[2] J.C. Halpin, Jn. Comp. Mat. 3 (1969) 732-734

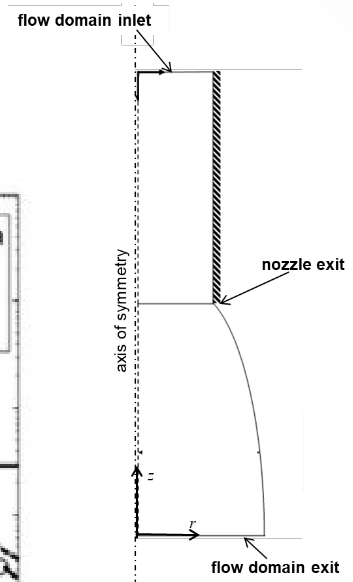
Polymer Composite Deposition Simulation

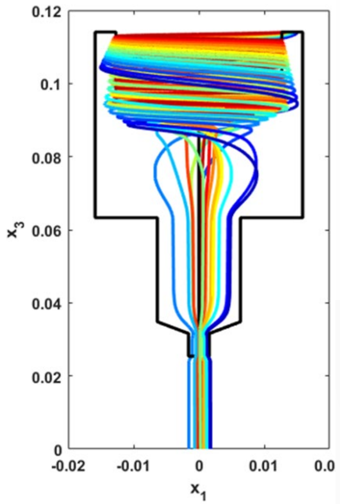


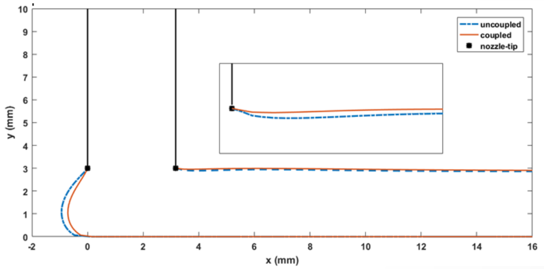
Polymer Melt Flow Models
2D and Axisymmetric flow
Stokes Flow
Isothermal & non-Isothermal
Incompressible
Creeping flow
Gravity, body forces, inertia ignored
Quasi-steady flow



Material Models
Newtonian
Power Law
Carreau-Yasuda
PTT (Visco-Elastic)







Free Surface Models
Die Swell (axismmetric)
Deposition (planar)

Software
ANSYS-Polyflow
COMSOL
MATLAB

Z. Wang, Z. Fang, Z. Xie, D.E. Smith, *Polymers* 14(22) (2022)
Z. Wang, D.E. Smith, *Comp. Part B*, 219 (2021) 108811
Z. Wang, D.E. Smith, D.A. Jack, *Add. Mfg.* 43 (2021) 102006
Z. Wang, D.E. Smith, *Materials*, 14(10) (2021) 2596
Z. Wang, D.E. Smith, *Comp. Part B.* 177(15) (2019) 107284
B. Heller, D.E. Smith, D.A. Jack, *Add. Mfg.* 25 (2019) 227-238
R. Russell, B. Heller, D.A. Jack, D.E. Smith, *Jn. Comp. Sci.* 2(2) (2018) 26
Z. Wang, D.E. Smith, *Jn. Comp. Sci.* 2(1) (2018) 10
B. Heller, D.E. Smith, D.A. Jack, *Add. Mfg.*, 12(B) (2016) 252-264

Bead Interface Healing Evaluation

- The principle of fusion bonding is commonly applied to the joining or welding of polymer melts which involves applying heat and pressure at the interface
- Degree of Healing D_h under isothermal conditions is written with respect to weld time t_w as [1]

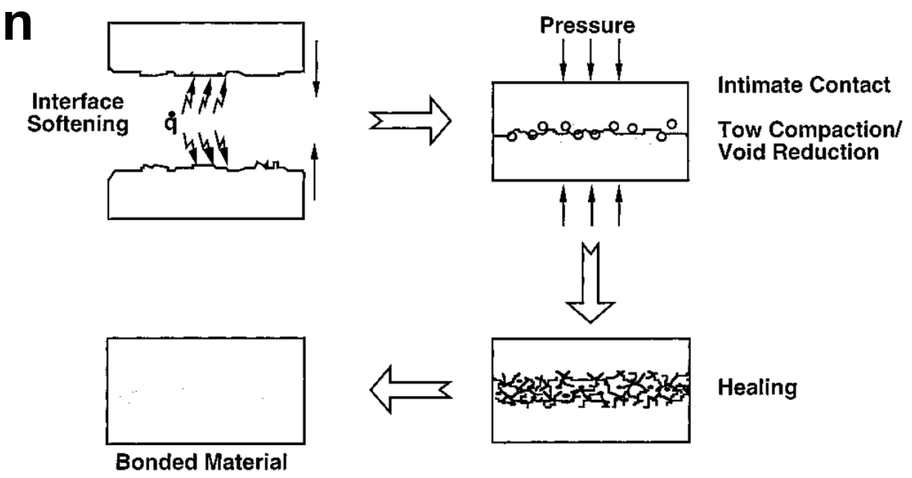
$$D_h(t) = \frac{\sigma}{\sigma_\infty} = \left(\frac{t}{t_w}\right)^{1/4}$$

- The above is extended to a non-isothermal degree of healing evolution with time as [2]

$$D_h(t) = \frac{\sigma}{\sigma_\infty} = \left[\int_0^t \frac{1}{t_w(T)}\,dt\right]^{1/4}$$

- Weld time t_w may be computed for ABS using experimental data from the literature ($Q_d = 388.7$ KJ/mol, R = universal gas constant) as [3]

$$t_w(T) = 1.080 \times 10^{-47} \exp\left(\frac{Q_d}{RT}\right)$$



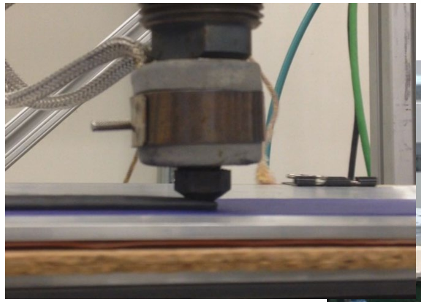
Taken from Yang and Pichumani [2]

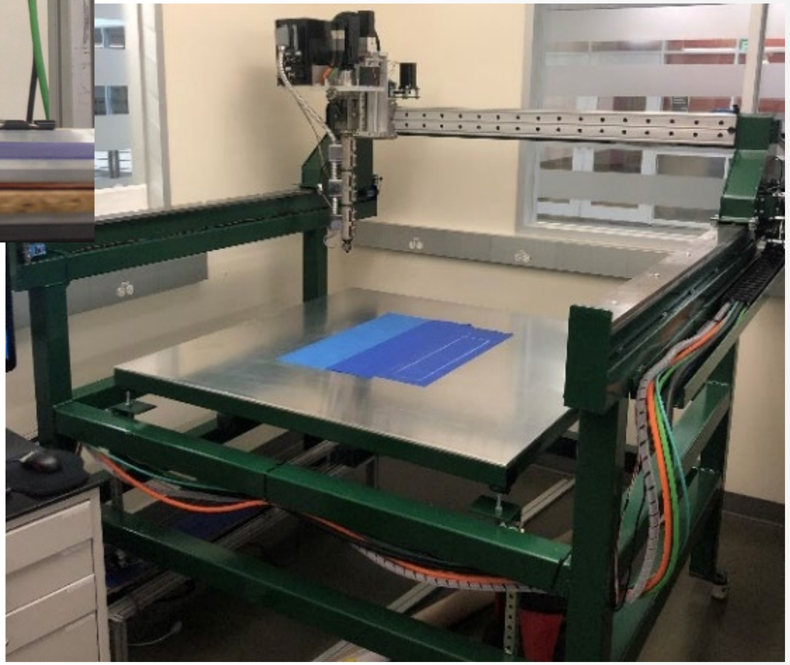
[1] R.P. Wool, K.M.. *Jn. Appl. Phys.*, 52 (1981) 5953-5963
[2] F. Yang, R. Pichumani, *Macromolecules*, 35 (2002) 3213-3224
[3] S.F. Costa, F.M. Duarte, J.A. Covas, *Jn. Mat. Proc. Tech.*, 245 (2017) 167-179

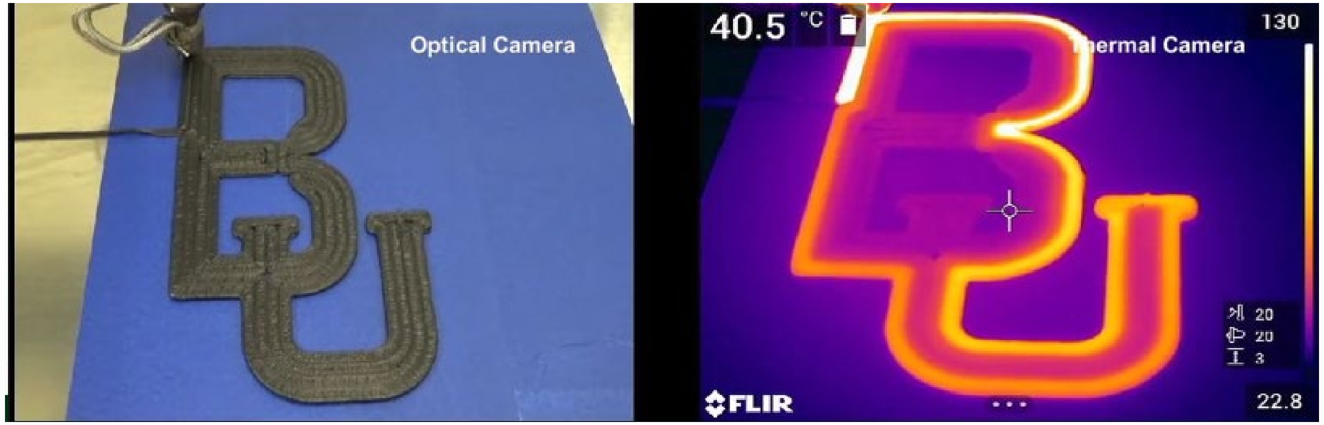
LAAM BEAD PREPARATION AND INSPECTION

Baylor Large Area Additive Manufacturing

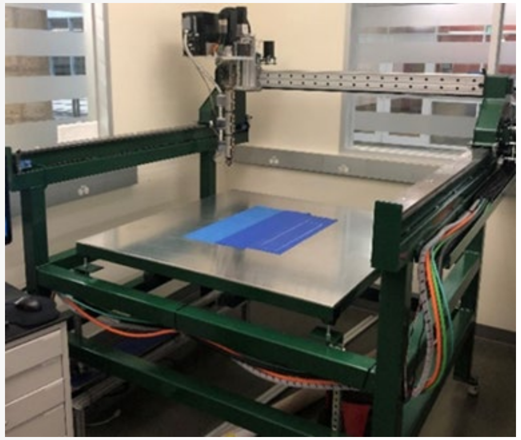
- Baylor LAAM
  - Print Bed: 4’ x 4’ x 6”
  - Deposition Rate: 19 lbs/hr
  - Nozzle Size: 0.125 and 0.25 inch
  - Input Material Format: Pellets
- Extruders:
  - Strangpresse Model 19 (ABS, PLA)
  - Dyze Design Pulsar (ABS, PLA, PEEK, PEI, TPE, TPU)







LAAM Sample Prep and Scanning



Baylor's LAAM system

parameter	value
temperature	220C
print height	2.5 mm
screw speed	90 RPM
nozzle diam	3.175 mm

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

Buehler IsoMet Low Speed saw

NSI X3000 micro-CT system
North Star Imaging, Rogers, MN, USA

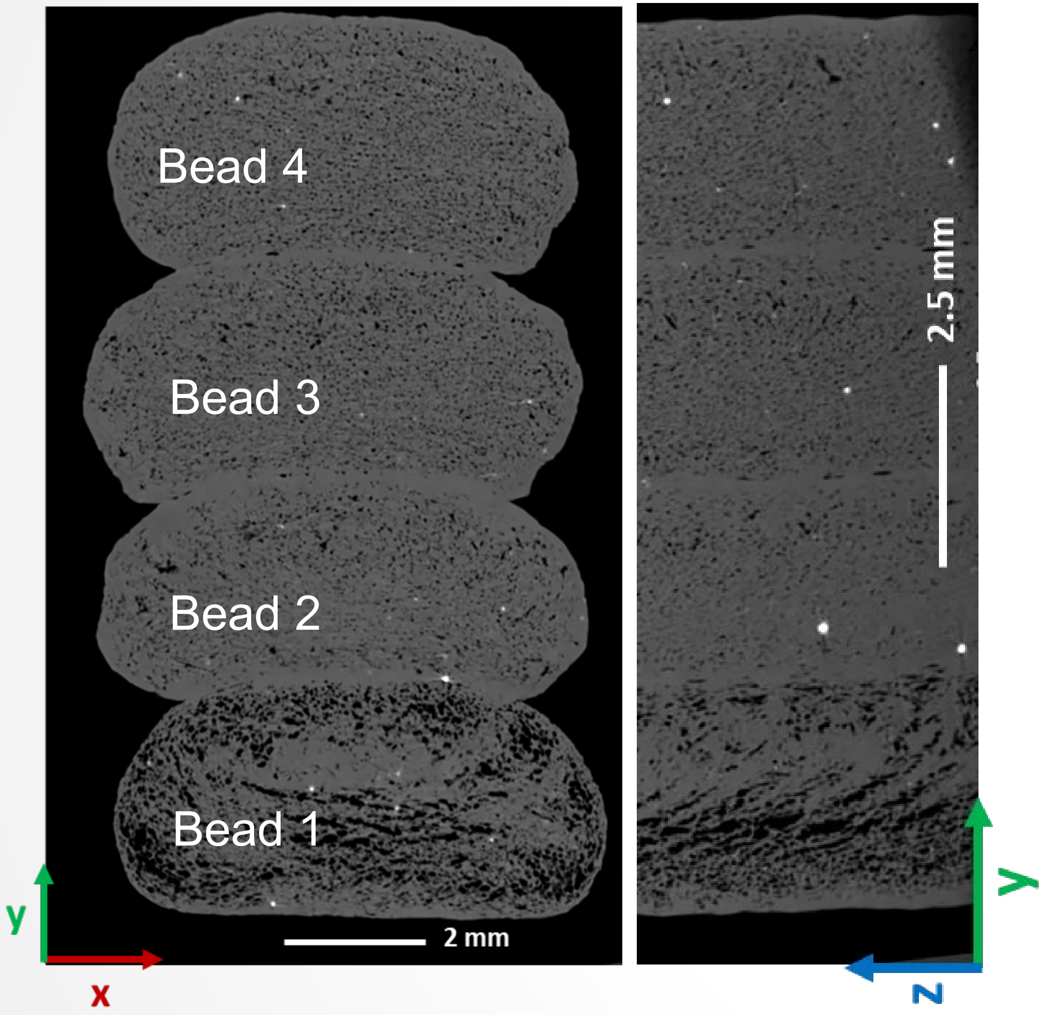
VOLUME GRAPHICS

NSI X3000 micro-CT scan parameters.

study	void	fiber
head	micro	nano
voltage	55 kV	60kV
current	80 μA	900 μA
resolution	10 μm	1.4 μm

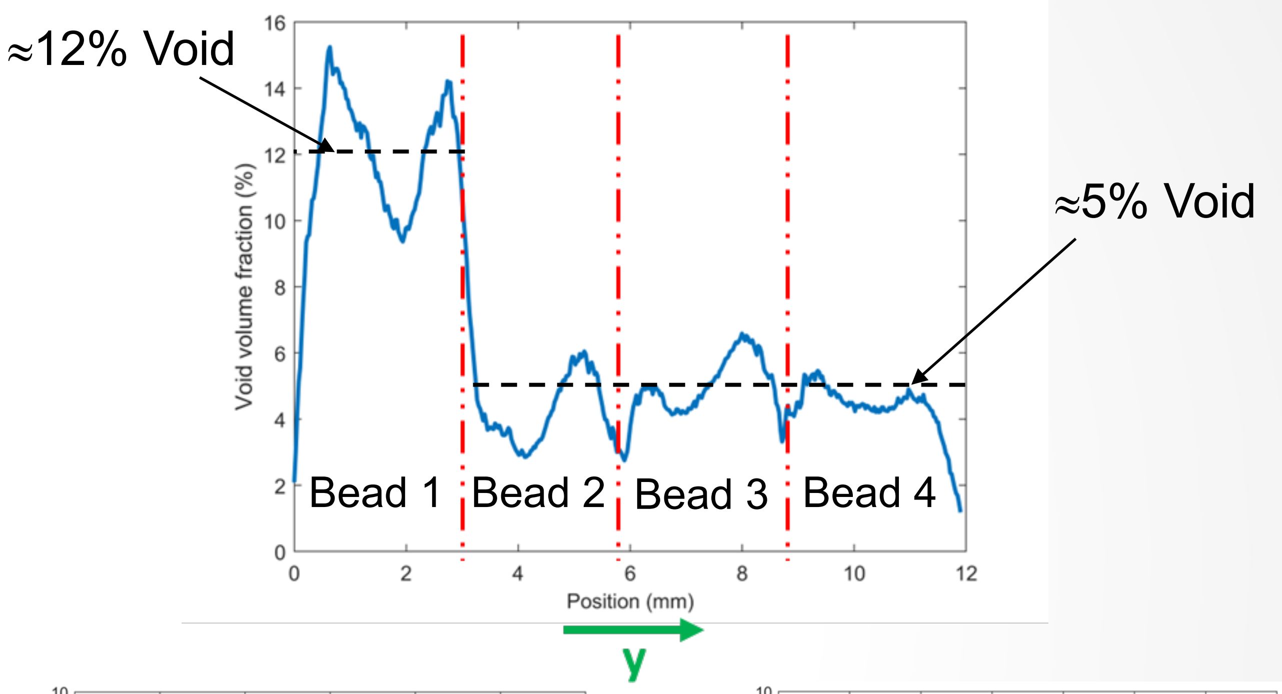
LAAM 4-Bead CF-ABS micro-Void Analysis

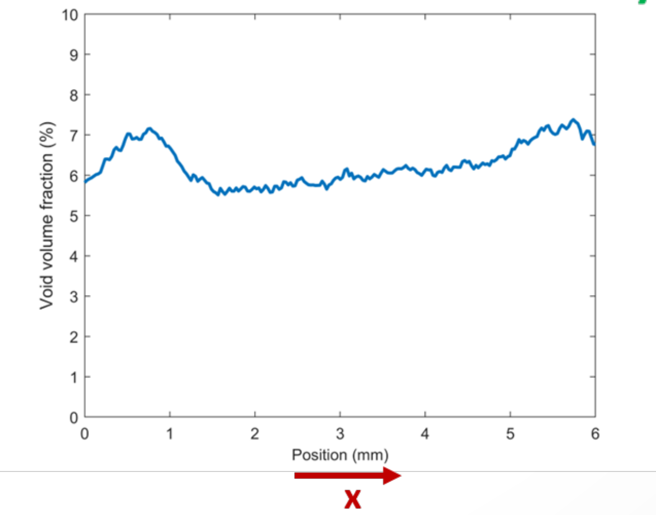
CF-ABS Single Bead Stack

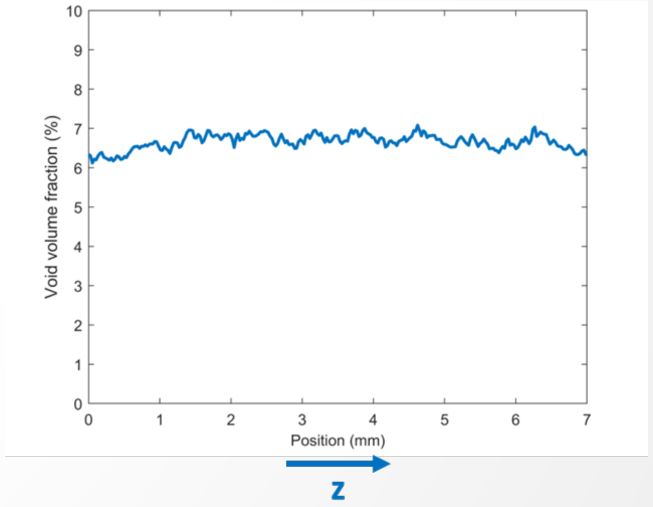


cross-X

side view

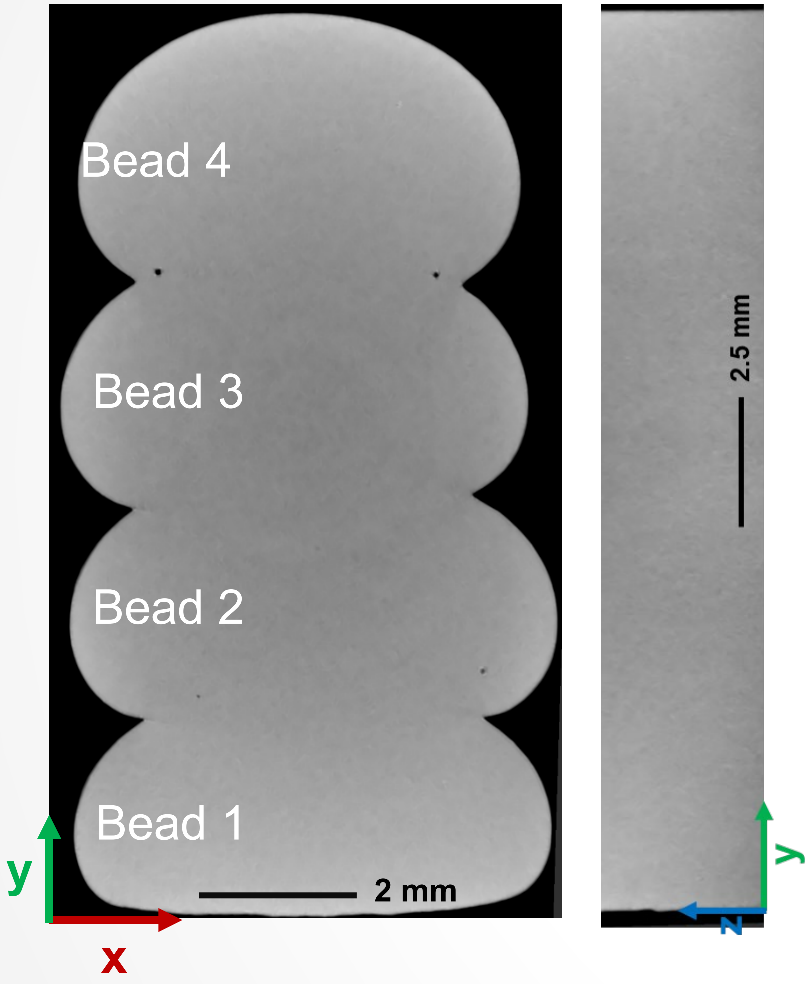






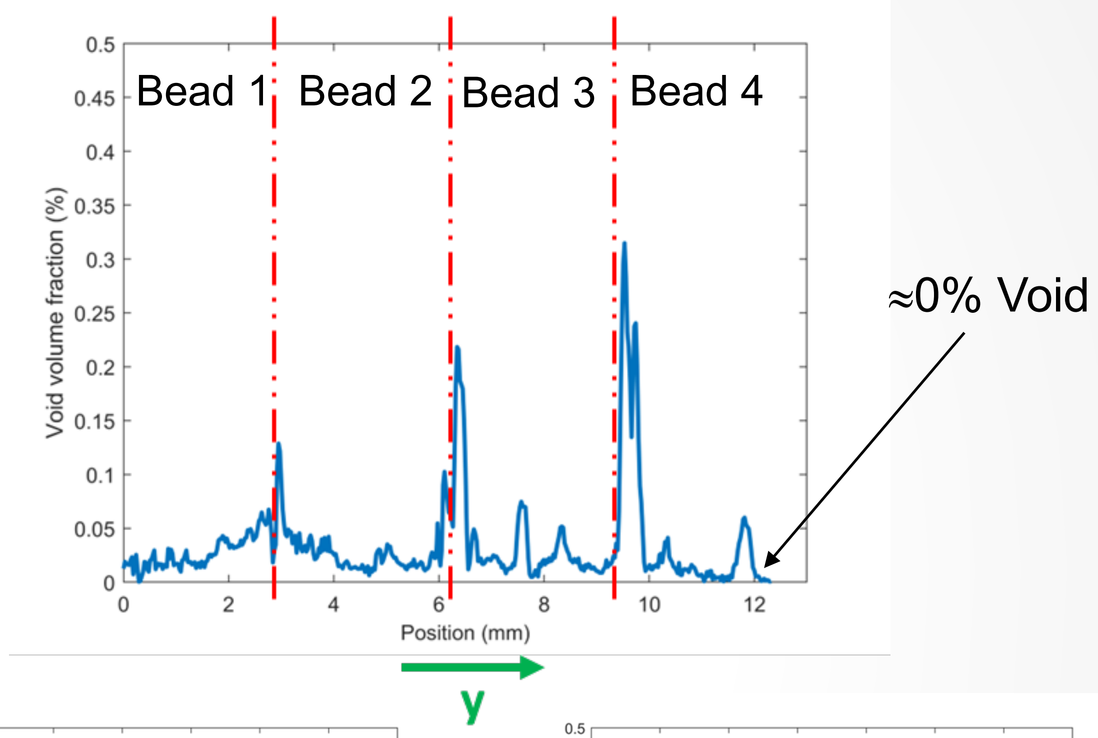
LAAM 4-Bead Neat ABS micro-Void Analysis

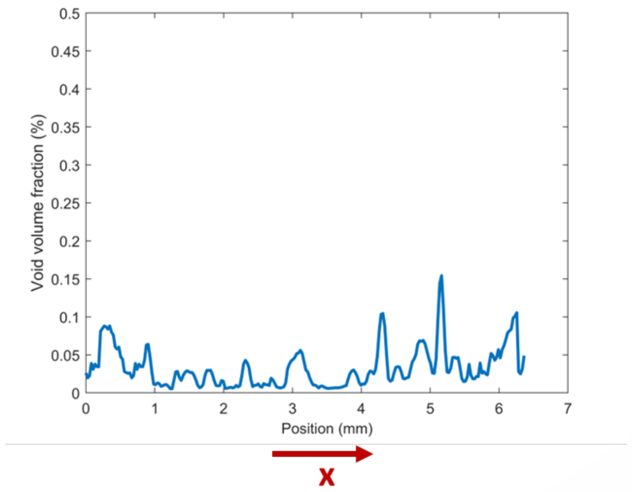
Neat ABS Single Bead Stack

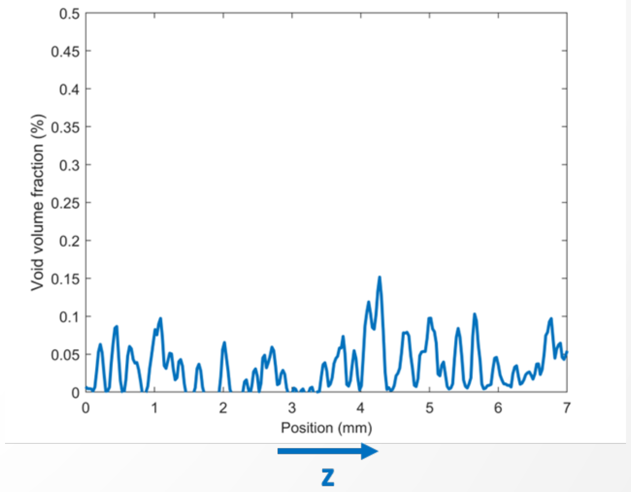


cross-X

side view



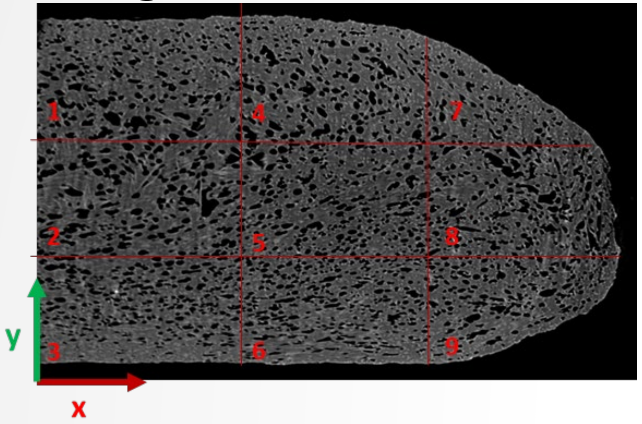


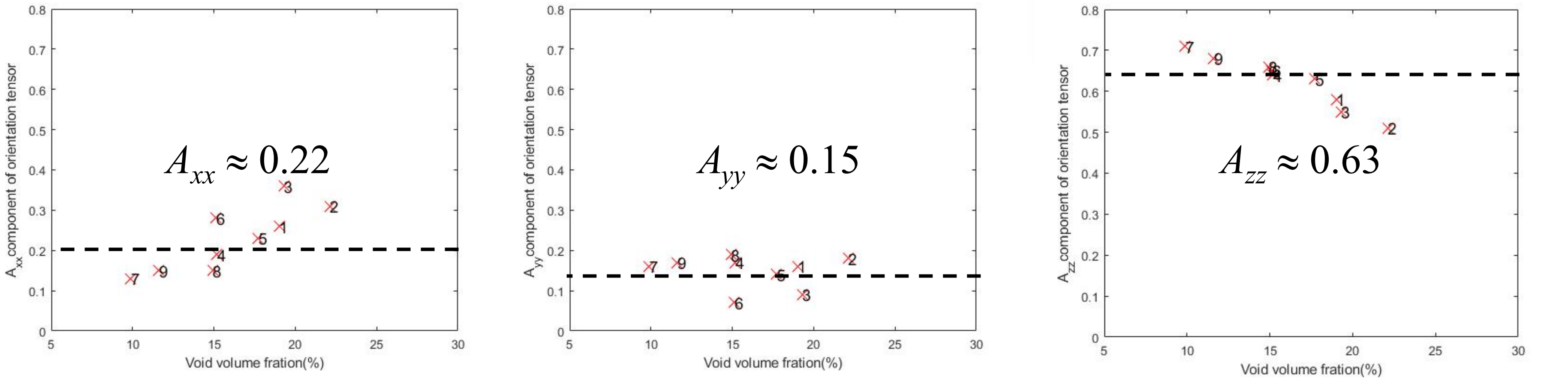


LAAM CF-ABS Fiber Orienation Analysis

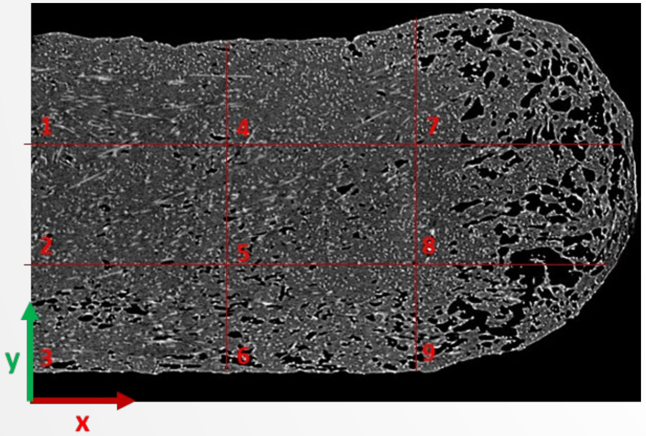
Fiber Orientation Tensor Diagonal Components

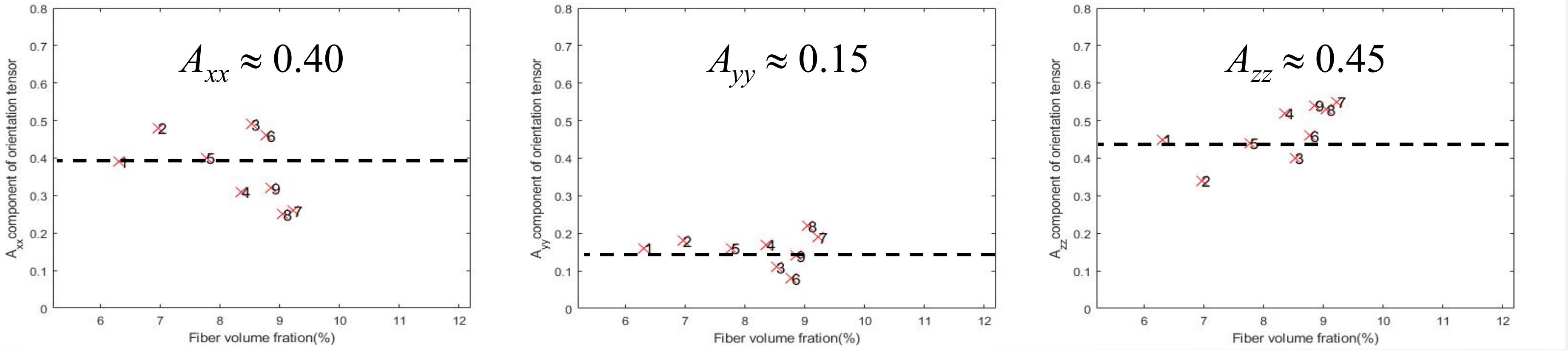
Single Bead As Printed





Single Bead Printed and Rolled

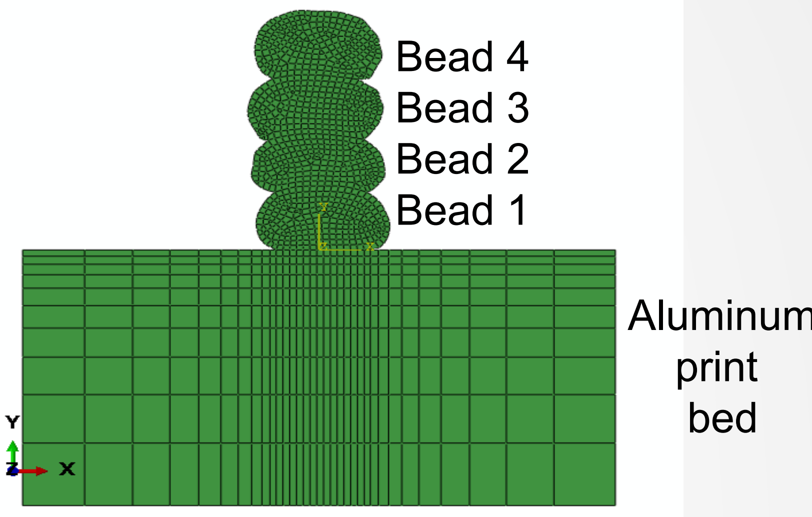




TRANSIENT THERMAL FEA

Transient Thermal FEA Model

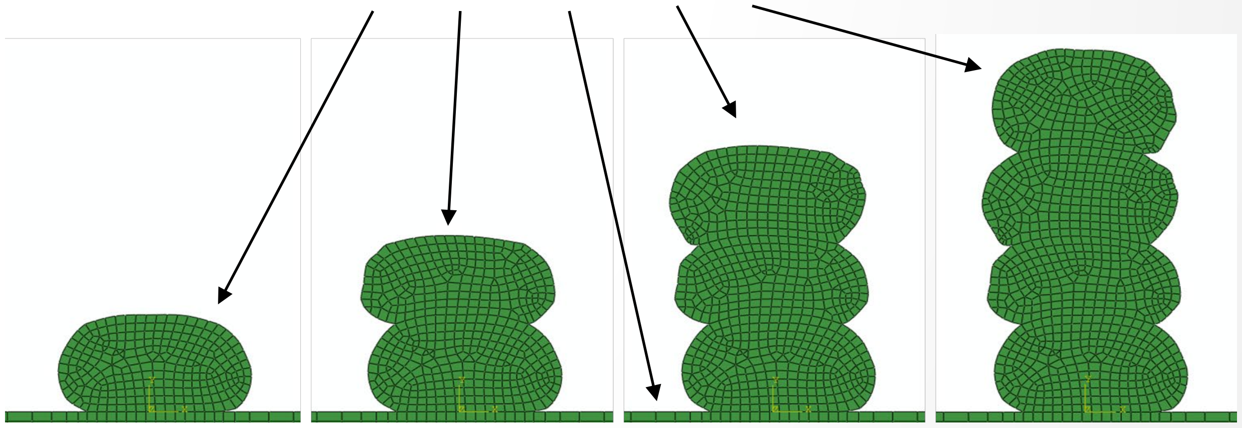
- **Single bead stack geometry taken from µCT scan data**
- **Linear transient thermal analysis performed in ABAQUS**
  - **2D heat transfer approximation**
  - **Element addition feature employed**
  - **Beads added at 17s intervals**
  - **Surface heat transfer applied to all external element edges**
  - **Conductivity computed from orientation tensors**
  - **Material properties scaled to account for intrabead voids**



- **Model Material Properties – literature values**

property	units	value
ABS conductivity	W/m-K	0.177
ABS heat capacity	J/g-K	2.08
ABS density	kg/m^3	1040
Carbon fiber conductivity	W/m-K	150
Carbon fiber heat capacity	J/g-K	1.15
Carbon fiber density	kg/m^3	1700

convection heat transfer, $h = 10$ W/m^{2}C



Simulation Cases Considered

CASE	SAMPLE	FIBER ORIENTATION	VOIDS
0	NEAT ABS	NONE	NO
1	CF ABS	ALIGNED	NO
2	CF ABS	ALIGNED	YES
3	CF ABS	UNIFORM	NO
4	CF ABS	UNIFORM	YES

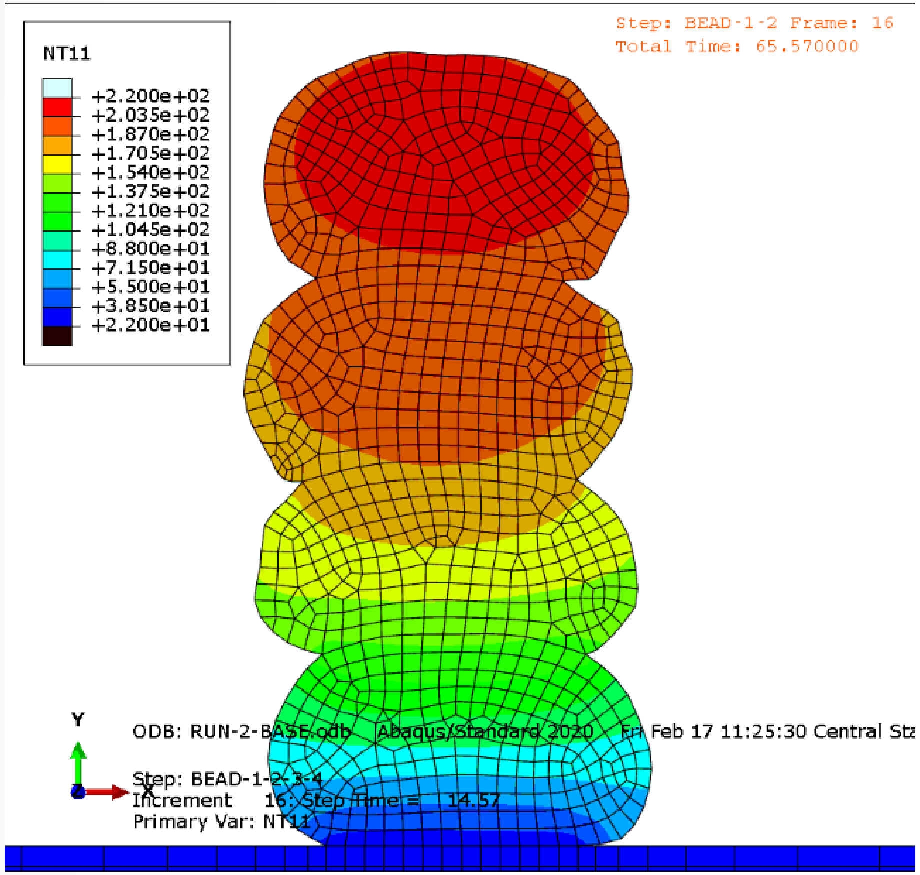
Aligned Distribution

$$A_{ij} = \begin{bmatrix} 0.125 & 0 & 0 \\ 0 & 0.125 & 0 \\ 0 & 0 & 0.75 \end{bmatrix}$$

Uniform Distribution

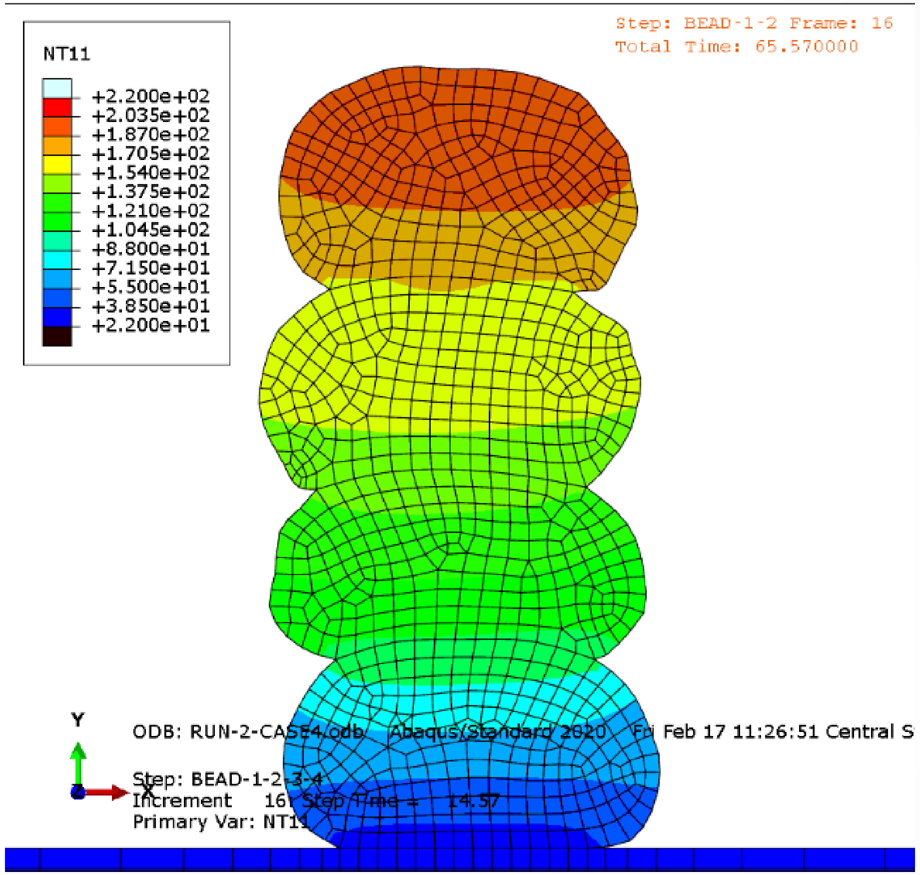
$$A_{ij} = \begin{bmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \end{bmatrix}$$

Transient Thermal FEA Bead Print Simulation



CASE 0: NEAT ABS

$k = 0.177$ W/m-K



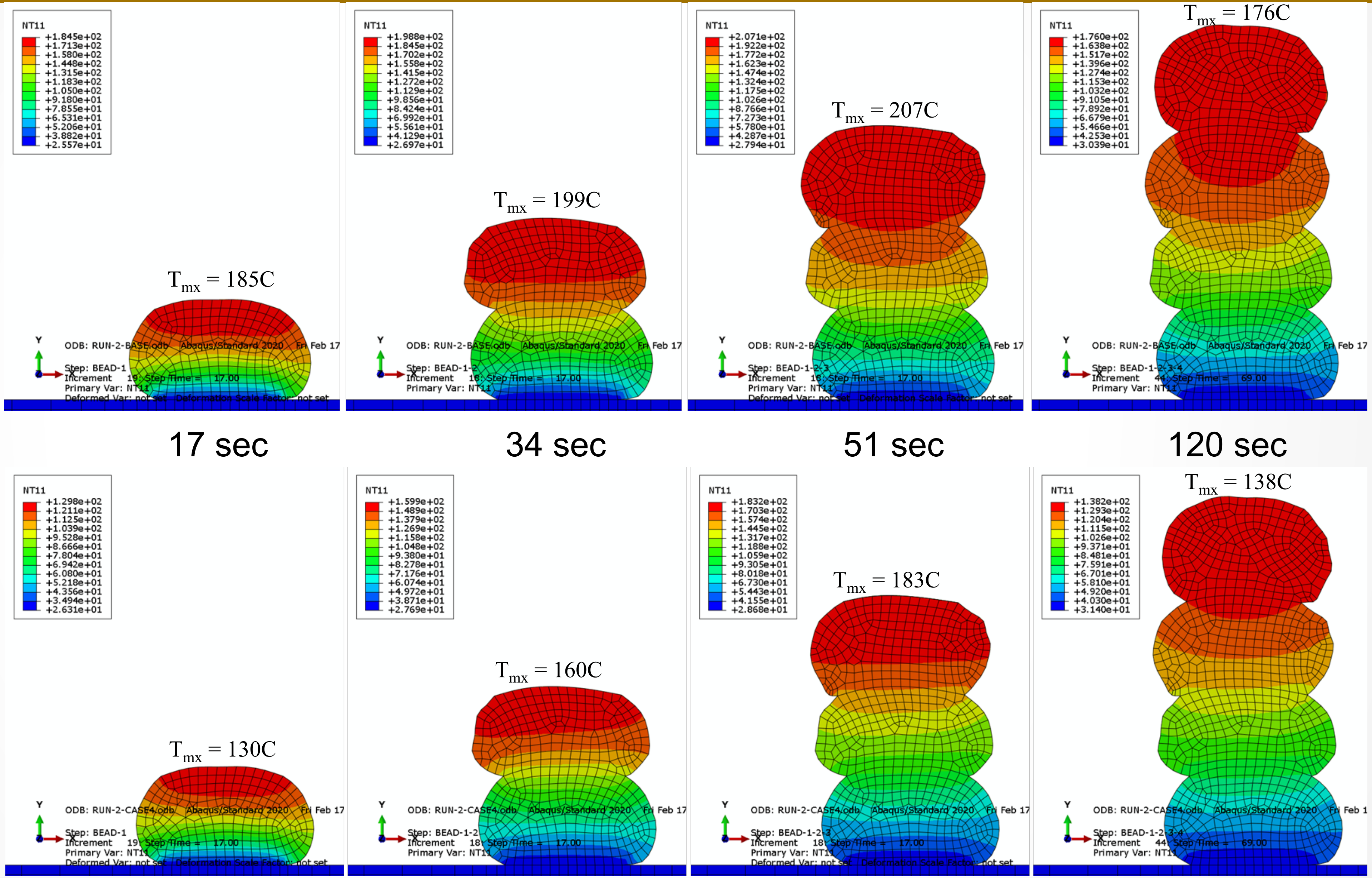
CASE 2: CFABS – ALIGNED - VOIDS

$k_{xx} = k_{yy} = 0.334$ to 0.361 W/m-K

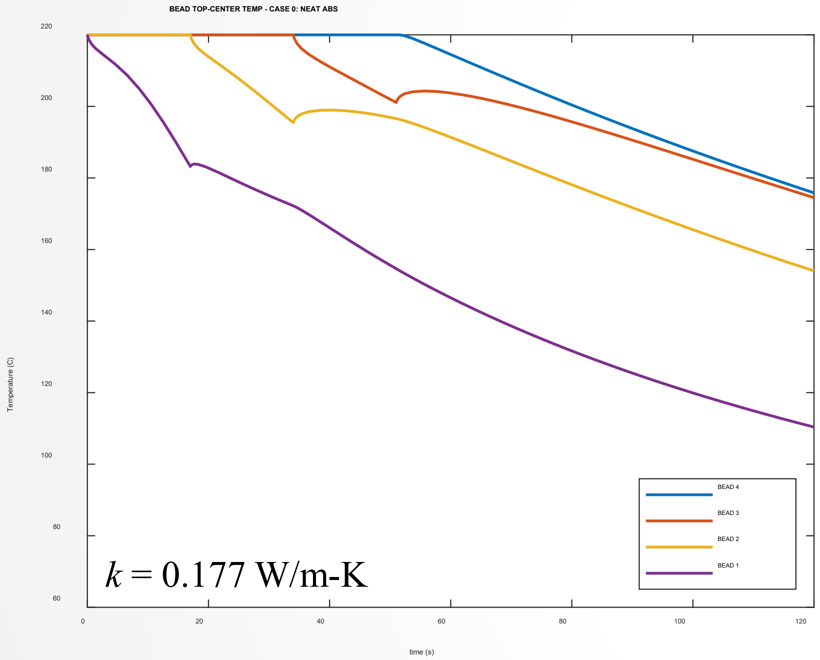
Temperature Prior to Next Bead Deposition

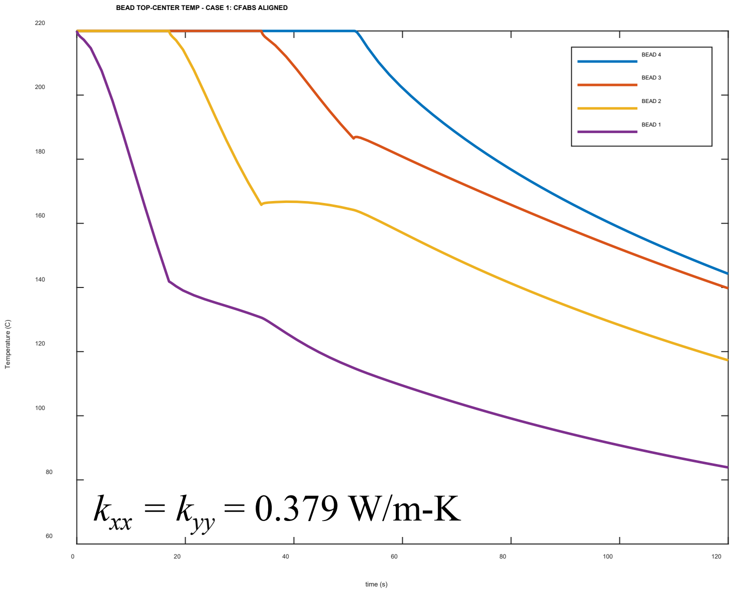
CASE 0: NEAT ABS

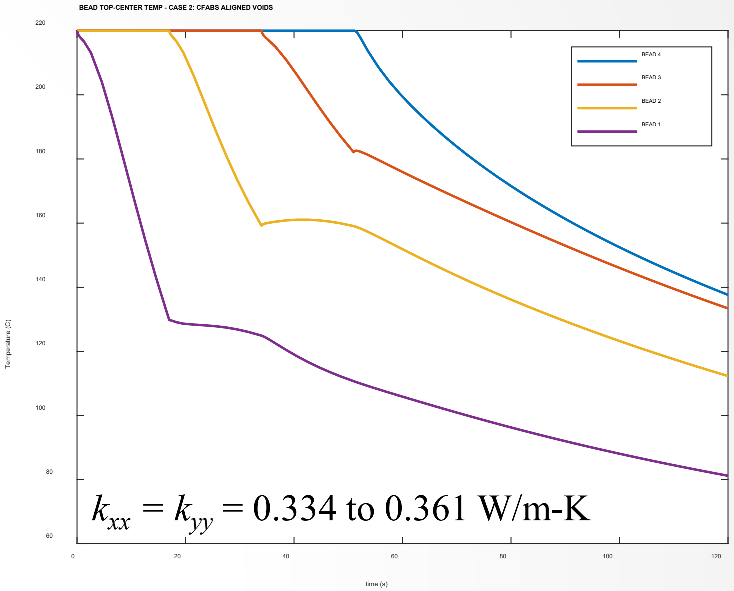
CASE 2: CFABS – ALIGNED - VOIDS

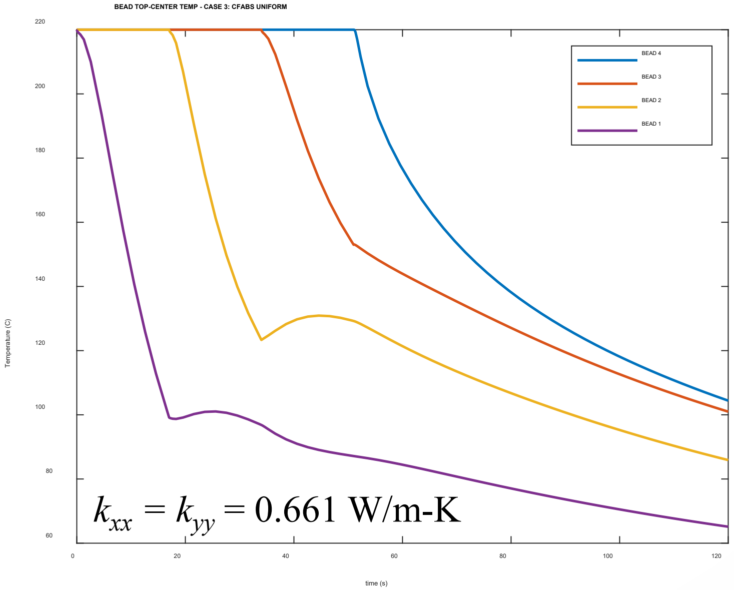


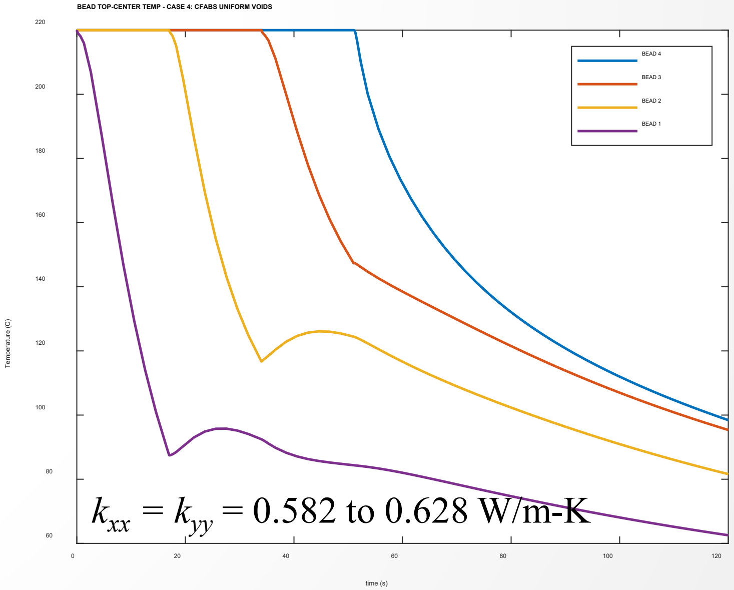
Bead Top-Center Temperature (°C)



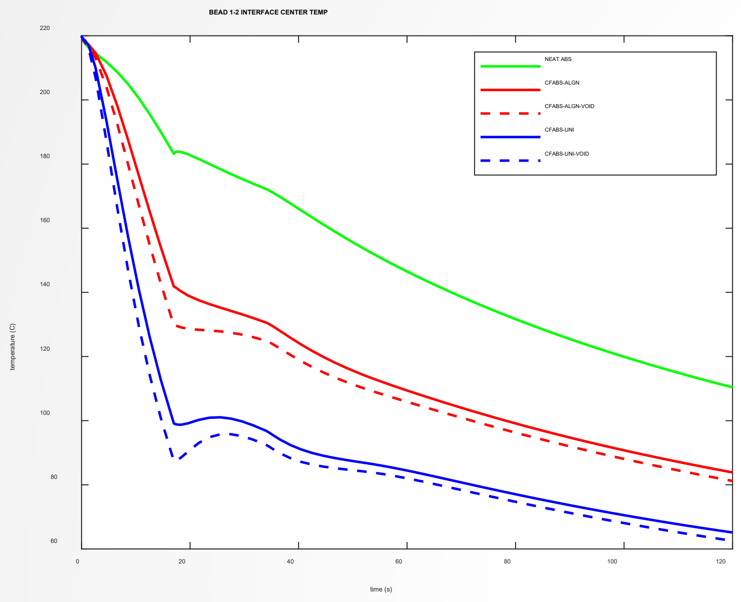


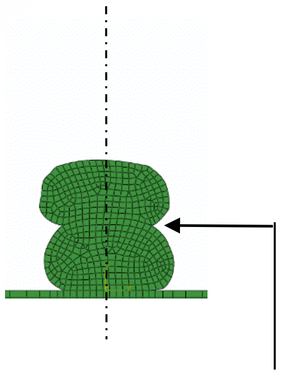




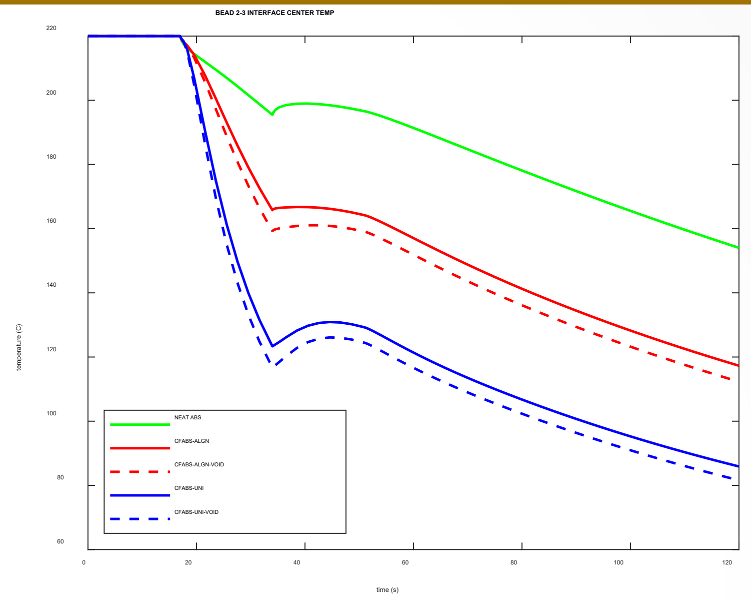


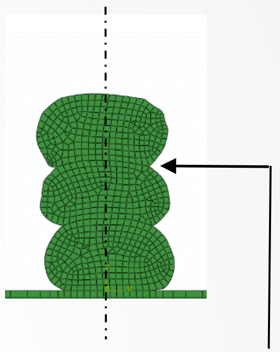
Bead Top-Center Temperature (°C)



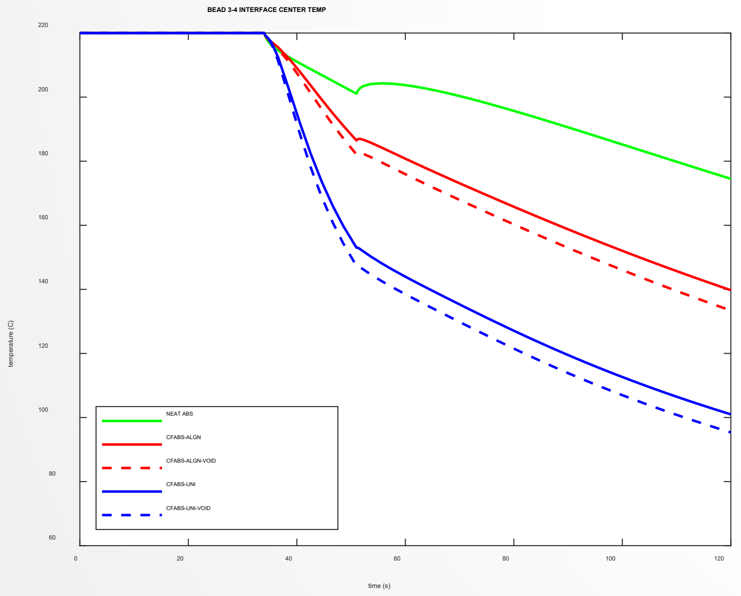


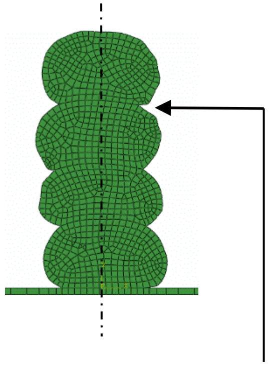
bead 1-2 interface



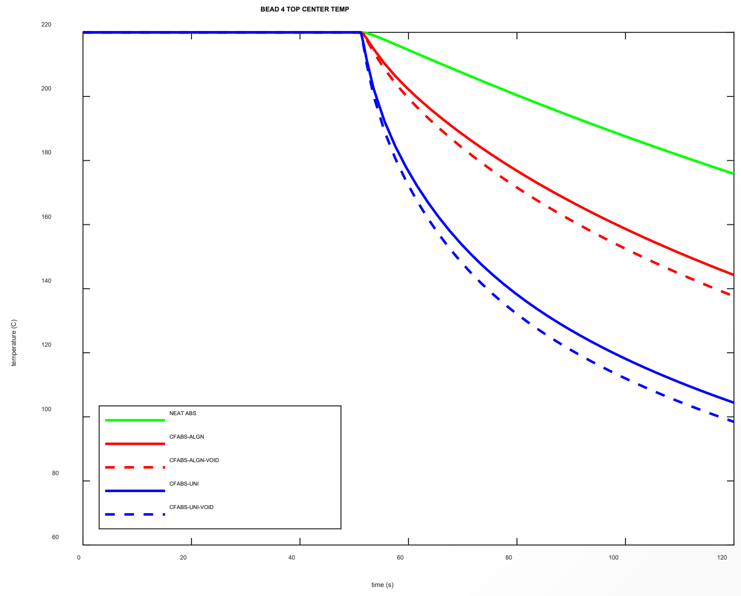


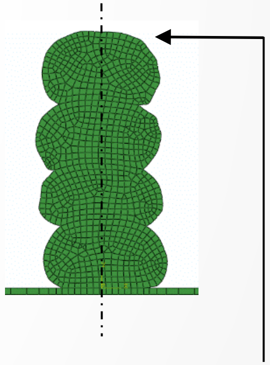
bead 2-3 interface





bead 3-4 interface





bead 4 top

Bead Top Center Temperature

Temperature just prior to next bead deposition

T (^oC) at $t = 120$s

CASE	SAMPLE	FIBER	VOID	BEAD 1	BEAD 2	BEAD 3	BEAD 4
0	NEAT ABS	NONE	NO	110.	154.	175.	176.
1	CF ABS	ALGN	NO	83.9	117.	140.	144.
2	CF ABS	ALGN	YES	81.2	112.	133.	138.
3	CF ABS	UNI	NO	65.1	85.9	101.	104.
4	CF ABS	UNI	YES	62.5	81.6	95.4	98.4

decrease thermal conductivity (mostly) ↑

increased distance from print bed →

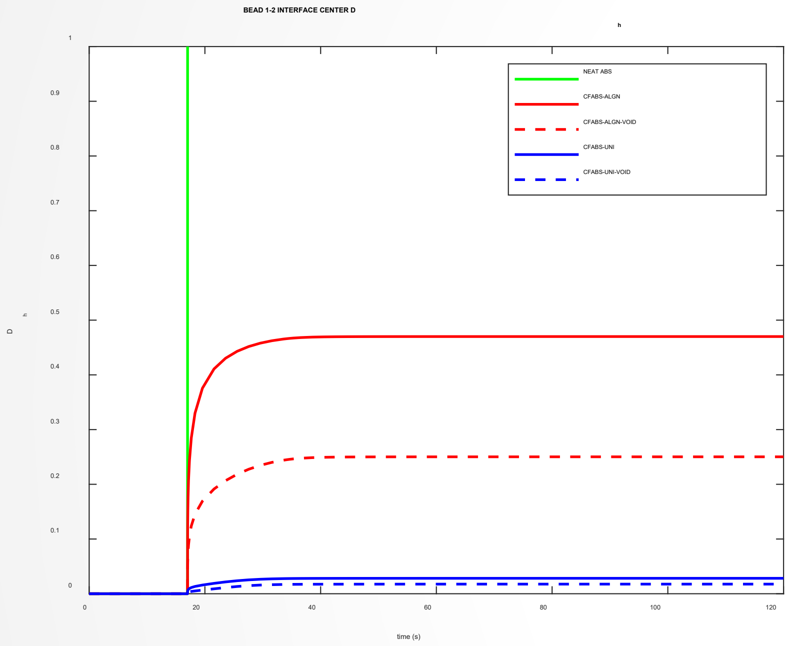
OBSERVATIONS

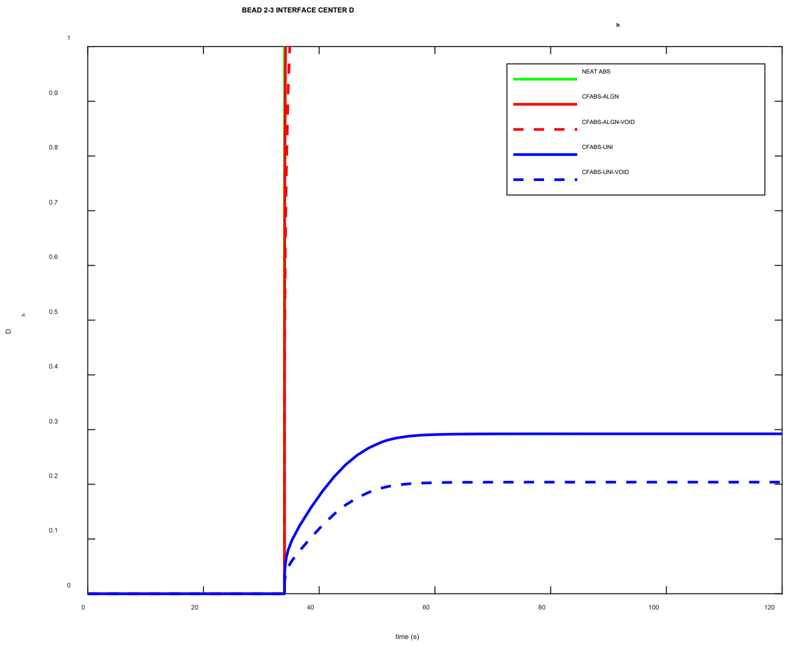
Neat ABS retains heat longer
Increased conductivity from carbon fiber increases heat transfer into print bed
Higher alignment along bead → Increased bead temperature
Voids tend to decrease bead temperature

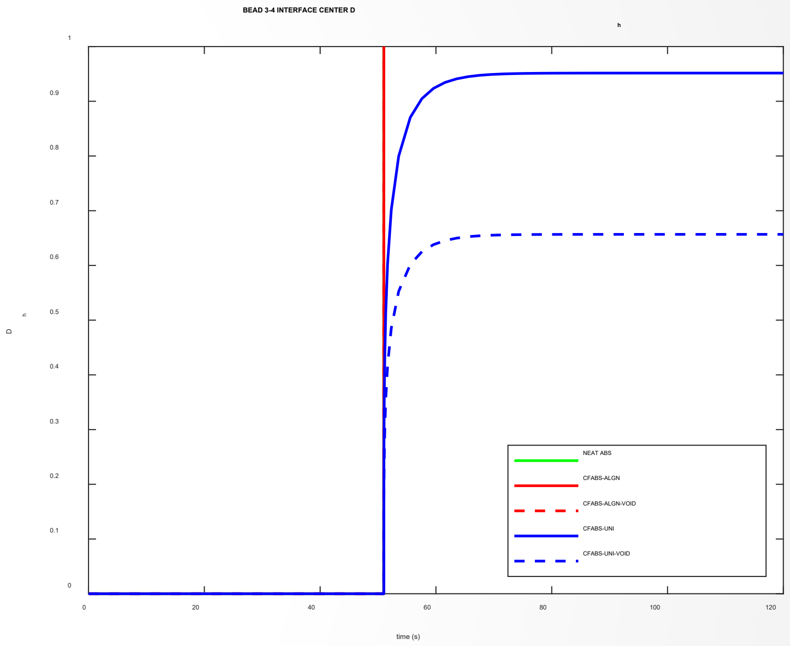
ADHESION ASSESSMENT

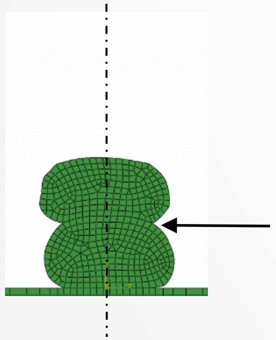
Bead Centerline Interface D_h

$$D_h(t) = \frac{\sigma}{\sigma_\infty} = \left[\int_0^t \frac{1}{t_w(T)}\,dt\right]^{1/4}$$

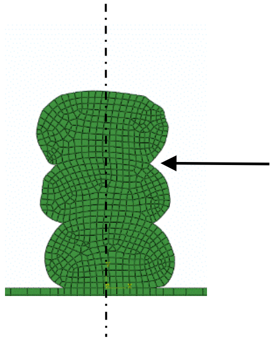




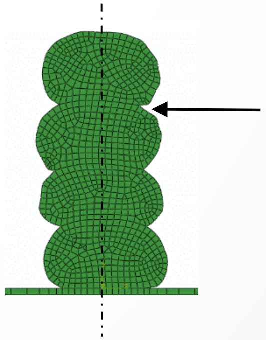




bead 1-2 interface



bead 2-3 interface



bead 3-4 interface

Bead Interface Center D_h

D_h at $t = 120$s

CASE	SAMPLE	FIBER	VOID	BEAD 1-2	BEAD 2-3	BEAD 3-4
0	NEAT ABS	NONE	NO	7.1	21.	27.
1	CF ABS	ALGN	NO	0.47	3.3	8.3
2	CF ABS	ALGN	YES	0.25	2.3	6.4
3	CF ABS	UNI	NO	0.028	0.29	0.95
4	CF ABS	UNI	YES	0.018	0.20	0.66

decreased thermal conductivity (mostly)

increased distance from print bed

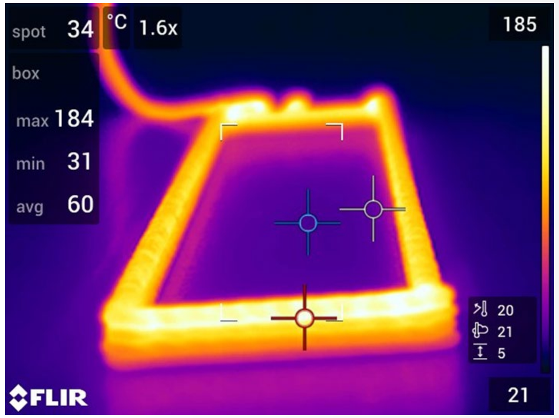
OBSERVATIONS

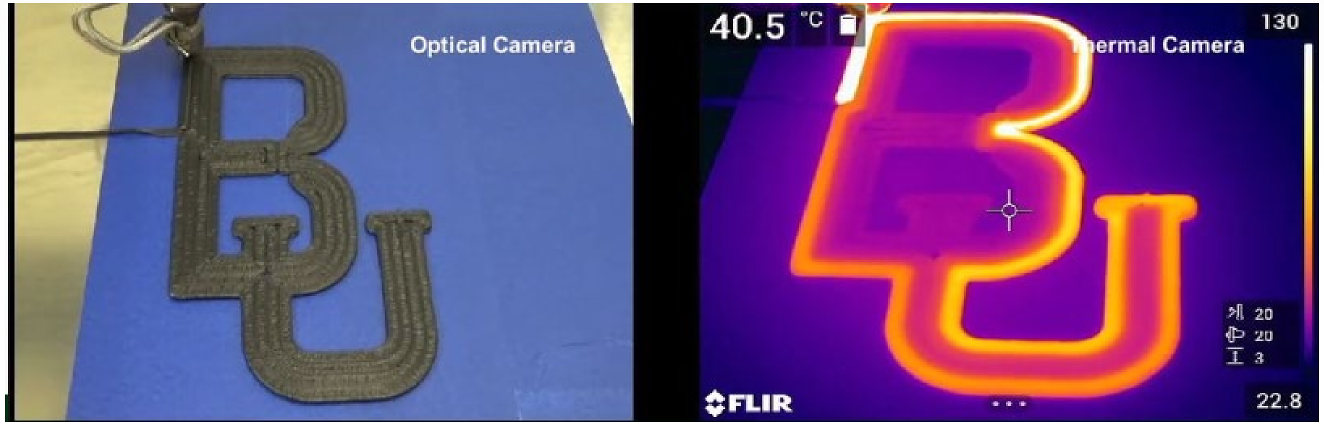
Increased adhesion further from print bed
Neat ABS has highest likelihood of adhesion
Increased transverse conductivity → Decreased likelihood of adhesion
Higher fiber alignment along bead → Increased likelihood of adhesion
Voids tend to decrease likelihood of adhesion

CONCLUSIONS

Conclusions

- Interlayer adhesion continues to be a limiting factor in adoption of large scale polymer composite deposition parts
- Single bead stack FEA simulations provided insight into cooling and adhesion
  - Carbon fibers increase cooling of bead stack
  - Higher fiber alignment along print bead improves adhesion
  - Adhesion enhanced with prolonged high temperature
  - Increased likelihood of adhesion away from print bed
  - Intralayer voids have less impact but tend to decrease likelihood of adhesion
- Future investigations should include experimental validation, additional beads, bead arrays, orientation tensor variation across bead, heat transfer coefficient identification, additional processing parameters, etc..





THANK YOU!

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