Lecture 6 - Orientation Averaging

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schedule

- 3 Feb - Orientation Averaging (HW1 Due)
- 8 Feb - Physical measurements
- 10 Feb - Variational Calculus (HW2 Due)
- 15 Feb - Variational Calculus

outline

- orientation averaging
- closure approximations

orientation average

orientation tensor

- Within a given volume, a distribution of fibers can be defined by some orientation distribution function, $\psi(\theta, \phi)$.
- Advani and Tucker introduced tensor representations of fiber orientation distribution functions

$$a_{ij} = \oint p_i p_j \psi(p) dp$$

orientation tensor

- And

$$a_{ijkl} = \oint p_i p_j p_k p_l \psi(p) dp$$

- Note: any order tensor may be defined in this manner, the orientation distribution function must be even, due to fiber symmetry, and thus any odd-ordered tensor will be zero.

orientation averaging

- Consider $T(p)$ to be some tensor property of a material, as a function of material orientation
- The orientation average of $T(p)$ is denoted by angle brackets and is given by

$$\langle T \rangle = \oint T(p)\psi(p)dp$$

orientation averaging

- For a uni-directional fiber, we would expect $\langle T \rangle$ to be transversely isotropic, which for a second-order tensor requires

$$\langle T_{ij} \rangle = A_1 \langle p_i p_j \rangle + A_2 \delta_{ij}$$

- but $\langle p_i p_j \rangle$ is the second-order orientation tensor
- The unknown constants, A_1 and A_2, can be easily solved for in terms of the uni-directional properties

orientation averaging

- Similarly, if T is a fourth-order tensor property then transverse isotropy requires that

$$\begin{aligned}\langle T_{ijkl}\rangle = B_1 a_{ijkl} + B_2(a_{ij}\delta_{kl} + a_{kl}\delta_{ij}) + \\ B_3(a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}) + \\ B_4(\delta_{ij}\delta_{kl}) + B_5(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\end{aligned}$$

- We can solve for B_α by considering fibers aligned in the three-direction, we have $a_{3333} = 1$ and all other $a_{ijkl} = 0$.
- We can choose any values of i, j, k, l that would give 5 unique equations to solve equations for B_α

orientation averaging

- Here we will consider T_{1111}, T_{3333}, T_{1122}, T_{2233}, T_{1313}.

$$\begin{aligned}T_{1111} &= B_4 + 2B_5 \\ T_{3333} &= B_1 + 2B_2 + 4B_3 + B_4 + 2B_5 \\ T_{1122} &= B_4 \\ T_{2233} &= B_2 + B_4 \\ T_{1313} &= B_3 + B_5\end{aligned}$$

orientation averaging

- After some manipulation, we find

$$
\begin{aligned}
B_1 &= T_{1111} + T_{3333} - 2T_{2233} - 4T_{1313} \\
B_2 &= T_{2233} - T_{1122} \\
B_3 &= T_{1313} - \frac{1}{2}(T_{1111} - T_{1122}) \\
B_4 &= T_{1122} \\
B_5 &= \frac{1}{2}(T_{1111} - T_{1122})
\end{aligned}
$$

closure approximations

closures

- While theoretically any-order orientation tensor is possible, in practice only the second-order tensor is used
- Microscopic measurements do not give enough information for higher-order tensors to be useful
- Software simulations have not implemented the fourth-order tensor
- To predict stiffness, we need the fourth-order tensor
- Closure Approximations are a way to approximate the fourth-order tensor from the second-order tensor

linear closure

- For 3D orientations, the linear approximation is given by

$$a_4^l = -\frac{1}{35}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) +$$
$$\frac{1}{7}(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{kl}\delta_{ij} + a_{jl}\delta_{ik} + a_{jk}\delta_{il})$$

- For planar orientations we simply replace the two coefficients with $-\frac{1}{24}$ and $\frac{1}{6}$

quadratic closure

- We can also use a quadratic closure method

$$a_4^q = a_{ijkl}$$

- If the fibers are randomly aligned, the linear closure will give the exact result
- If the fibers are perfectly oriented, the quadratic closure will give the exact result

hybrid closure

- Advani proposed a hybrid closure to take advantage of both the linear and quadratic methods
- We will introduce a parameter f and use it to combine both linear and quadratic closures

$$a_4^h = (1 - f)a_4^l + fa_4^q$$

- Ideally, we would like f to be 1 for perfectly oriented fibers and 0 for random fibers

hybrid closure

- Advani proposes

$$f = A a_{ij} a_{ji} - B$$

- Where $A = 3/2$ and $B = 1/2$ for 3D orientations and $A = 2$ and $B = 1$ for planar orientation

orthotropic fitted closure

- A more recent method that is commonly used is known as the orthotropic fitted closure
- The fourth-order tensor is approximated in the principal direction, then rotated back out if necessary

orthotropic fitted

- In the principal direction, the fourth-order tensor will be orthotropic (represented in 6x6 as)

$$A_4 = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 & 0 \\ A_{12} & A_{22} & A_{23} & 0 & 0 & 0 \\ A_{13} & A_{23} & A_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & A_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & A_{66} \end{bmatrix}$$

orthotropic fitted

- The symmetry of the orientation tensor requires that A_{66} (which is a_{1212}) be equal to A_{12} (which is a_{1122})
- By the same symmetry, we have $A_{55} = A_{13}$ and $A_{44} = A_{23}$.
- We also know that $a_{ijkk} = a_{ij}$, which imposes the following equations:

orthotropic fitted

$$A_{11} + A_{66} + A_{55} = a_{11}$$
$$A_{66} + A_{22} + A_{44} = a_{22}$$
$$A_{55} + A_{44} + A_{33} = a_{33}$$

orthotropic fitted closure

- This leaves only three independent variables in the fourth-order tensor that need to be found.
- Different authors have proposed different functions to fit these three independent variables
- They are fit to give the best mold simulation predictions, but do not necessarily have any physical application

discrete calculations

- To compare with our laminate analogy we can calculate the orientation tensor for discrete orientation states

$$a_{ij} = \frac{1}{N} \sum p_i p_j$$

for second-order tensors and

$$a_{ijkl} = \frac{1}{N} \sum p_i p_j p_k p_l$$

example

- Compare Mori-Tanaka stiffness predictions for direct calculation and orientation averaging
- Compare $[0/90]_S$, $[\pm 45]_S$, and $[0/\pm 45/90]_S$
- link[1]
- Also compare the results with a closure approximation of the fourth-order tensor

[1]https://colab.research.google.com/drive/1PpahfEvGbXo6P22jI_o0FCFUYOjmpQ3n?usp=sharing