Using Material Designer To Perform Homogenization Studies



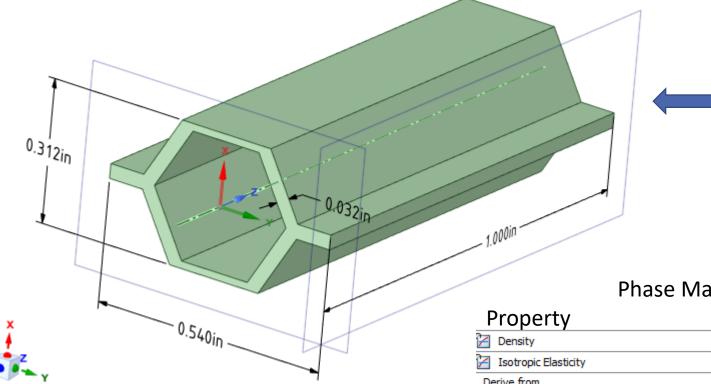
Mechanical Material Homogenization: An Overview

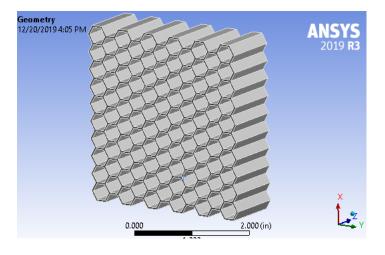
- Engineers commonly find that they have to simulate parts and assemblies with composite or fine lattice structures
- Typically, such structures consist of a 'unit cell' repeated many times in one or more spatial directions
- This unit cell is often much smaller than the overall structure under investigation. So much smaller, in fact, that it is impractical (or impossible) to model it in detail
- The solution in such cases is a technique called "homogenization", in which the unit cell structure is considered independently. The goal is to determine the effective, or average elastic properties of the unit cell. Assuming the unit cell is uniformly repeated over the domain of an entire structure, the effective constitutive properties of the unit cell will characterize the entire domain as well
- The result is an orthotropic stiffness matrix, which can then be incorporated into larger structures as a material property
- In the past, one could perform such a study manually.
- Starting at release 19.2, ANSYS introduced Material Designer, which is a much simpler and more efficient workflow. We will discuss this workflow, and assess its accuracy using a 'real-world' model problem



The Model Problem: A Uniform Honeycomb Structure

• We consider a three dimensional honeycomb structure having unit cell dimensions and phase material properties below





Phase Material: Nylon 12

Property	Value .	Unit
Density	0.033598	lb in^-3
Isotropic Elasticity		
Derive from	Young's Modulus and Poisson's Ratio 📃	
Young's Modulus	2.4656E+05	psi
Poisson's Ratio	0.394	
Bulk Modulus	3.8768E+05	psi
Shear Modulus	88438	psi



The Model Problem (continued)

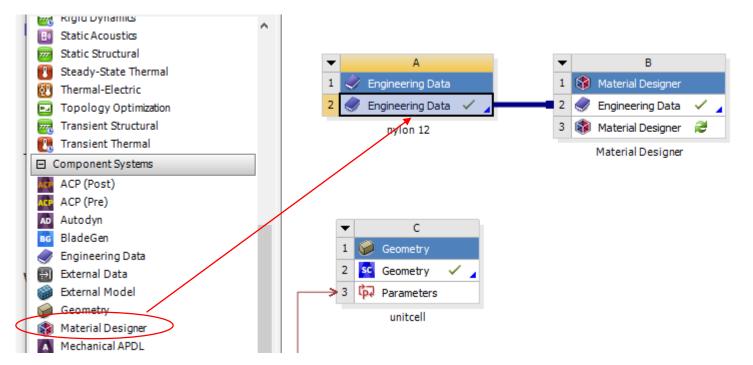
- The end-goal is to be able to replace the honeycomb structure with 'homogenized' (effective) material properties
- Since Material Designer doesn't have a hexagonal unit cell built-in, we've created the unit cell in SpaceClaim and we will import it as a user-defined unit cell
- Since we won't give Material Designer any additional symmetry information, we expect a full orthotropic stiffness matrix with nine independent entries:

$$\mathbf{\underline{C}} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}$$



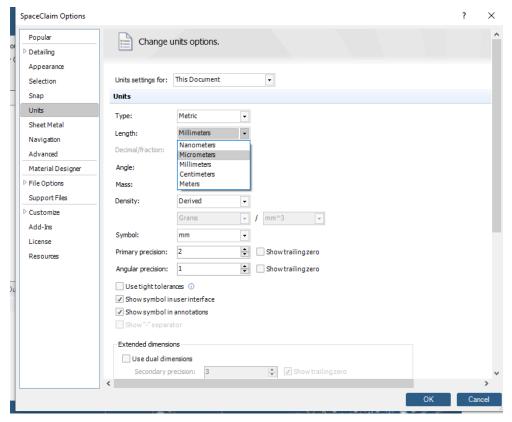
The Procedure

- As Material Designer is still considered a beta feature, some of the usual Workbench project operations are not yet available. For example, we can't just drag and drop a Material Designer (MD) object from the toolbox onto a Geometry cell. There are some additional subtleties which we'll cover in a moment.
- Begin by Defining a new MD system in the Project Schematic. Do this by dragging and dropping the new system onto an Engineering Data cell containing the phase material(s)



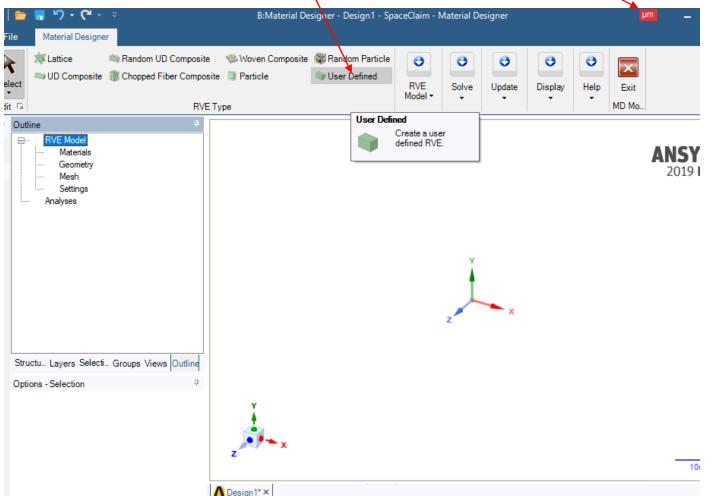


- Open an MD window (double-click or edit the MD cell).
- Since we're going to import the geometry, MD requires us to first set the units to 'microscale' manually. This is very important! If you don't do this, MD will refuse to import the model (and not tell you why). Do this by clicking the File tab->SpaceClaim Options (MD is actually a SpaceClaim plug-in). Navigate to Units, and select Micrometers



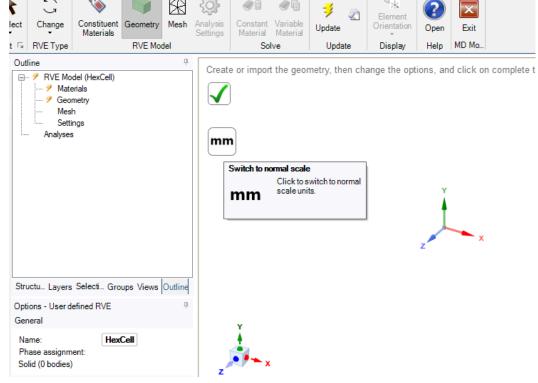


- You should now see the small red " μ m" icon in the upper right
- Next, click 'User Defined' under RVE Type



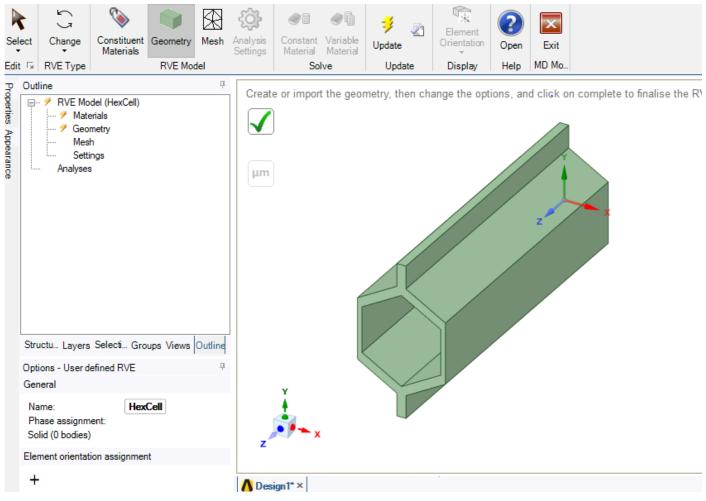


- Next, name your RVE (Representative Volume Element)
- Name all phases (we only have one. Voids aren't considered phases)...
- Now, click on 'Geometry' in the RVE Model group (and reset the 'name' of the RVE if you have to!)
- IMPORTANT: Click on the 'mm' button to switch to normal scale. If you don't, MD won't let you import.



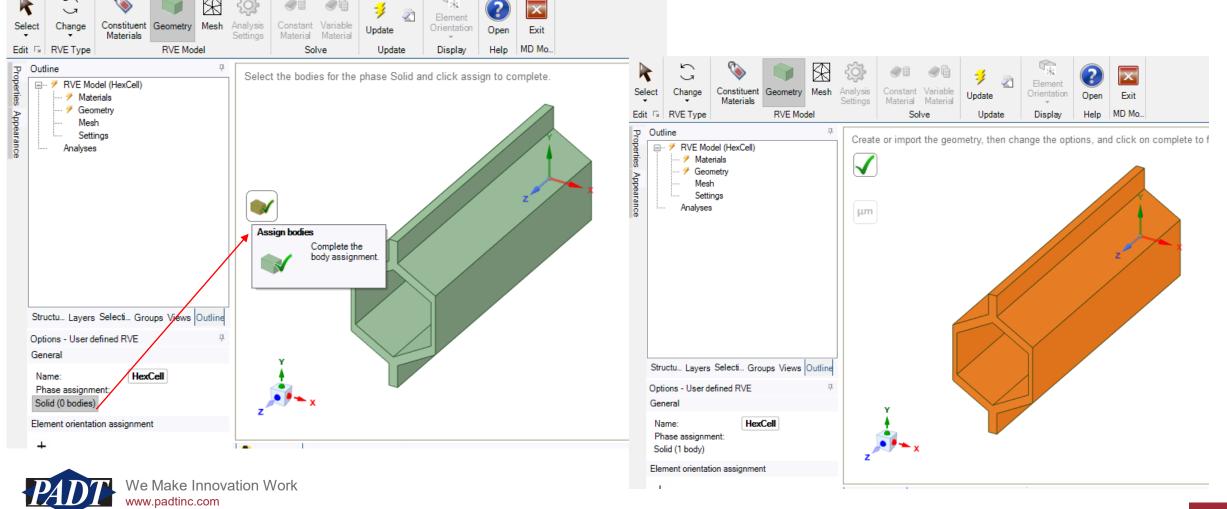


- In another window, open your SpaceClaim unit cell geometry
- Now, cut-and-paste the geometry from SpaceClaim into MD...

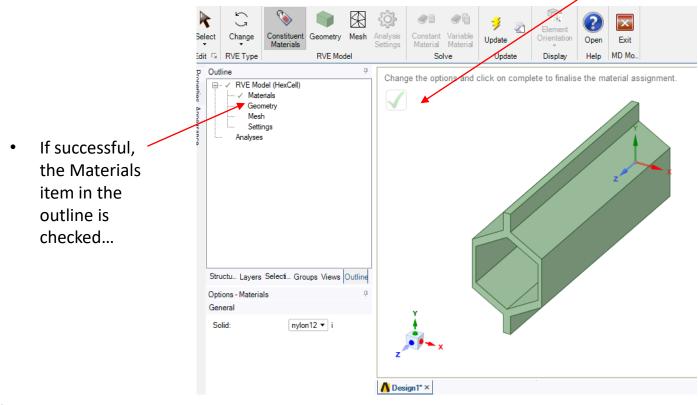




- Click on each phase name (in the lower left RVE Options window) to assign it. Again, we only have one, so we do this once
- Click the checkmark to finalize the RVE creation



- If successful, the Geometry item in the outline will be checked.
- Next, set the material, by selecting Constituent Materials in RVE Model group (we could have done this first. The order isn't important). Click the Checkmark to complete the Materials definition. Again, for composite unit cells, we could have multiple material assignments. We only have one.





 Next, select 'Mesh' in the RVE Model group. Note the settings in the Options window in the lower left. We're going to just accept all the default options because –except for the mesh size. In this example, I've typed in 0.5 mm (basically half the wall thickness of my unit cell). Click the checkmark

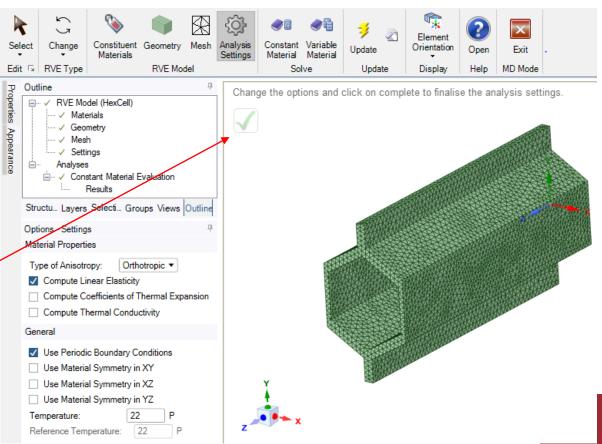
 If successful, you see a mesh, and the 'Mesh' item in the Outline is checked...

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elect Change	Constituent Materials	Geometry	Mesh	Analysis Settings		Variable Material	Update	Orientation	Open	Exit	
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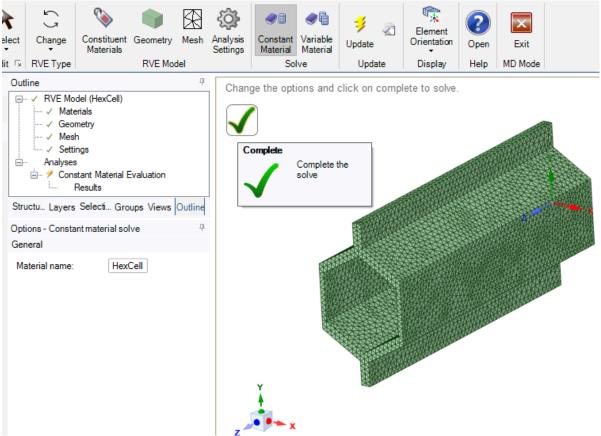


- The reader may have noticed that we're simply going from left-to-right in the RVE Model menu group. If we continue in this way, the next step is Analysis Settings. Note the options there
- At this point, we're going to accept all the defaults. Readers may argue that there is additional symmetry we
 can make use of, and they are correct. This, however, is the heart of this article, and we want to
 demonstrate what happens when one doesn't do this.
- We should also point out that what is meant by "Material Symmetry" here is not "model (unit cell) symmetry", but symmetry of the effective material we're trying to simulate (symmetry about orthotropic axes)
- Again, we're going to leave this question for later when we do a detailed validation of the properties we calculate
 - Hit the checkmark when done to accept





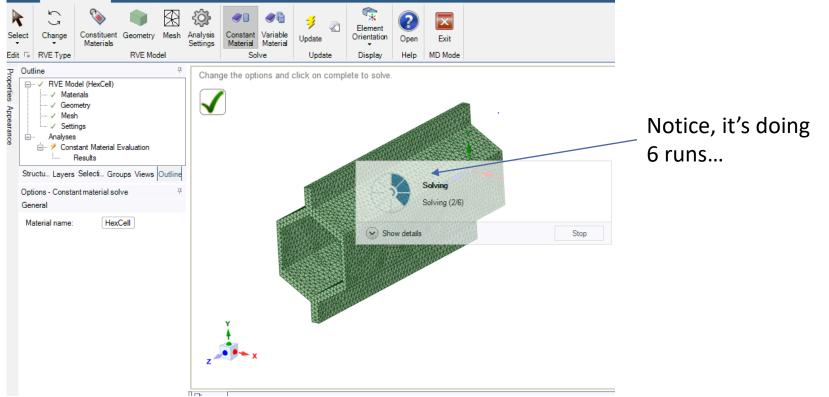
- We've now completed the RVE Model definition and defined the type of analysis we're going to do. The next step is to solve. Select 'Constant Material' under the 'Solve' group
- The the material a name
- Hit 'Complete the Solve' checkmark





The Procedure

- Since this is a three dimensional model, MD gives us nine independent material constants (three elastic moduli, three shear constants, and three Poisson ratios). Without any additional information, this requires six independent load cases (recall, we didn't use any additional symmetry options)
- The user can see this in the progress bar when solving...





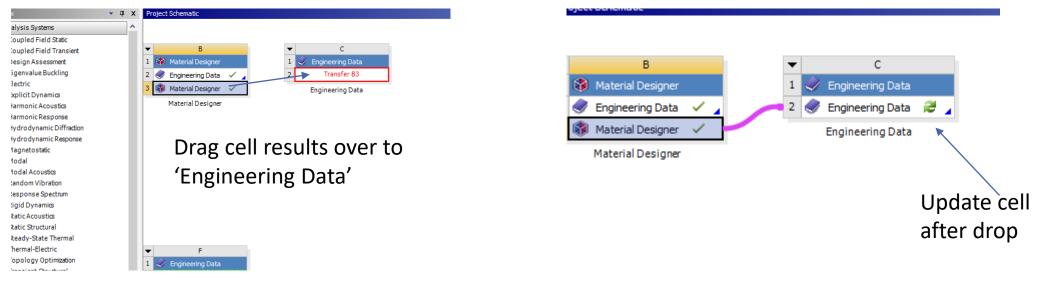
• When done, you'll be able to expand the Analysis item in the Outline and view the results

Sel	ect	Change	Constituent Materials	Geometry	Mesh	Analysis Settings	Constant Materia	⊘ ∎ Variable Material	誟 🖉 Update	Element Orientation	? Open	Exit	
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							nu23		0.039521				
							Density						
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Model Validation (cont.)

- At this stage of development, we don't seem to have much choice in selecting units when viewing our homogenized properties (we're stuck with N,mm). However, we can transfer these results to a new 'Engineering Units' object in the Project Schematic. This is something you'll probably want to do anyway (assuming you want to use the homogenized properties for a downstream study)
- Do so by dragging and dropping a new Engineering Data object onto the Project Schematic. Then use your left mouse button to drag the Material Designer cell over to the new Engineering Data object as shown below. Once complete, right-click on any cells which need to be refreshed or updated, and click 'Update' as necessary



Model Validation (cont.)

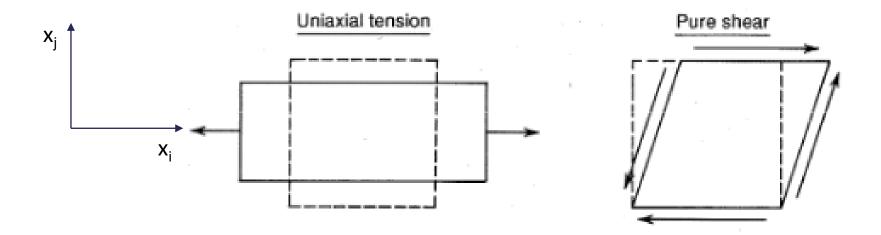
• Double-click (or right-click and 'Edit') the new 'Engineering Data' cell to view the orthotropic properties just calculated in the unit system of your choice

- Note the magnitude of v_{xy} (0.86!)
- This isn't unusual for composite materials or lattice structures, but we're still suspicious...
- So, let's try to validate these numbers "the old fashioned way"

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1 3 4 5 6 7 8	A Property Density Orthotropic Elasticity Young's Modulus X direction Young's Modulus Y direction Young's Modulus Z direction Poisson's Ratio XY Poisson's Ratio YZ Poisson's Ratio XZ					Value .0065431 718.7 718.6 8017 .86466 .030513 .030514	Unit Ib in^-3 psi psi psi	D	Е			



 A typical homogenized material property study for a 3-dimensional unit cell with no additional symmetries requires six separate load cases in order to obtain the nine independent coefficients. These consist of three mutually perpendicular tension/compression tests, and three mutually perpendicular pure shear tests

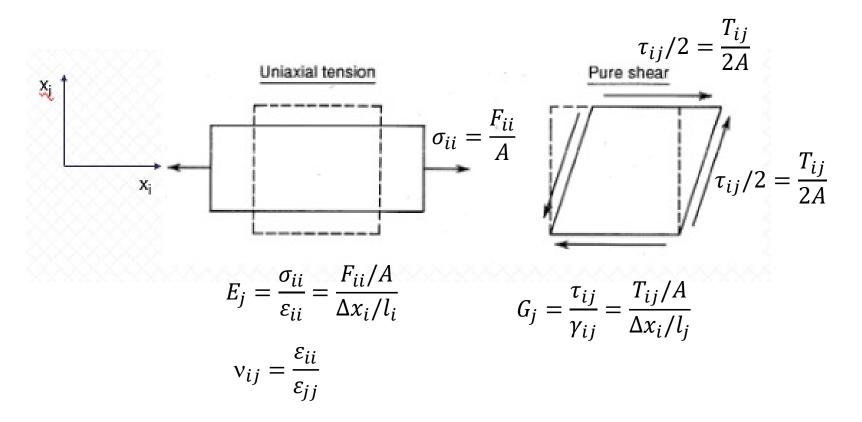


- The coordinate indices (I,j) above are the unique planar combinations of (x,y,z)
- In other words, the two tests above are performed in planes (x,y), (y,z), and (x,z)
- The three Poisson ratios may be obtained from the three uniaxial tension/compression tests. This is why we don't have to perform nine independent tests



- It's usually slightly simpler (and runs faster) to apply the load cases as applied displacements or strains, rather than as loads
- Doing so also simulates how such actual tests are performed, so that's how we'll apply the load cases
- So, in the uniaxial tension/compression tests, we apply a strain, δ of 5% (or γ = 0.05 in the case of shear). We will do this via displacements, scaled to the appropriate length of the unit cell
- For the pure shear case, we will apply a shearing displacement, $\gamma/2$ to two orthogonal planar faces (for each of the three planar cases), where γ is the total shearing displacement
- For all load orientations (except for loads ON the x-y plane), the boundary conditions consist of fixing faces parallel to the loaded faces in the direction of loading. Forces are determined by applying a force probe on the applied nonzero deflection faces
- Faces normal to these have periodic symmetry defined
- Finally, we will follow the previous assumption we made in Material Designer –there is no additional material symmetry to make use of...

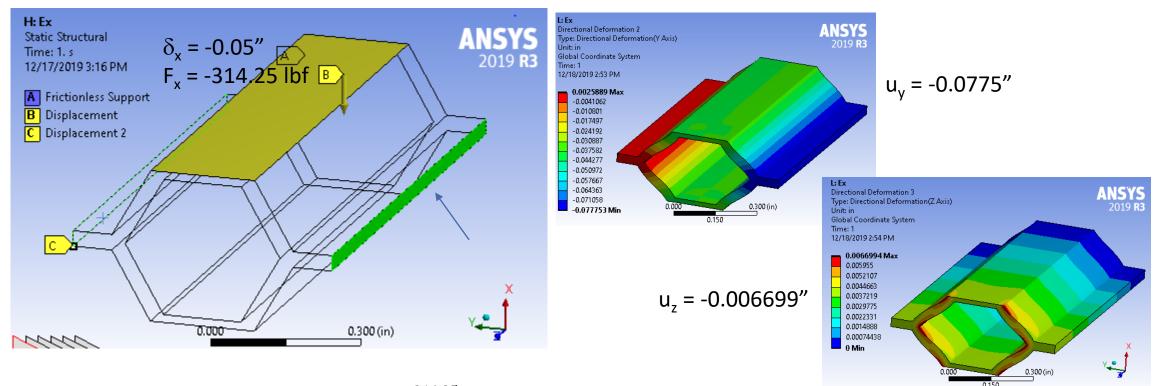




- In all cases, strains are applied as displacements $\Delta x/l$
- Forces and tractions are retrieved by force probe in Mechanical



Case 1: Uniaxial Tension (Y-Z plane)



Transverse deflections

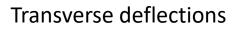
$$E_{\chi} = \frac{\sigma_{\chi\chi}}{\varepsilon_{\chi\chi}} = \frac{-\frac{314.25}{0.54*1.0}}{-0.05/0.31177} = 3692.165 \text{ psi}$$

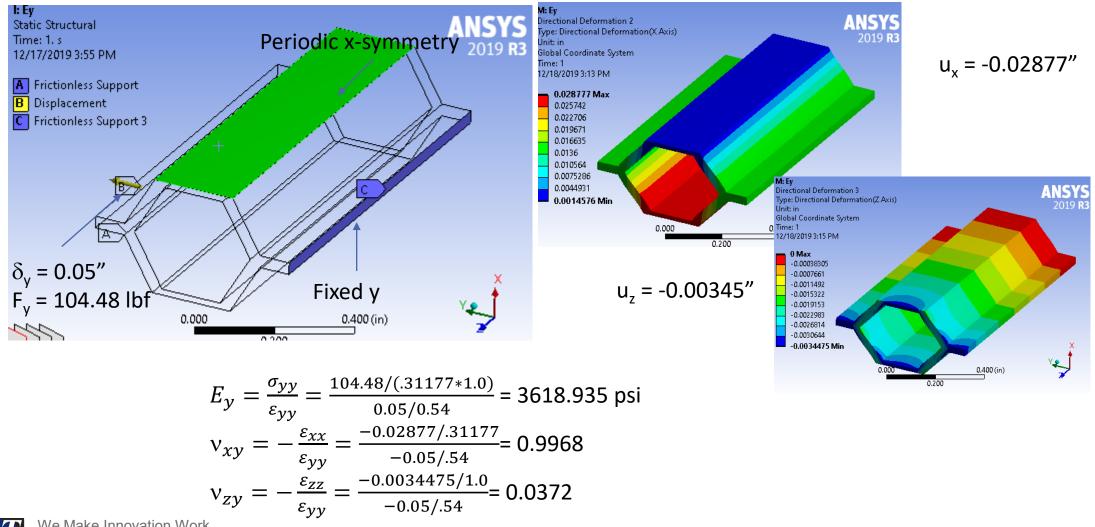
$$v_{\chi\chi} = -\frac{\varepsilon_{\chi\chi}}{\varepsilon_{\chi\chi}} = \frac{-0.0775/.54}{-0.05/.31177} = 0.895$$

$$v_{Z\chi} = -\frac{\varepsilon_{ZZ}}{\varepsilon_{\chi\chi}} = \frac{-0.006699/1.0}{-0.05/.31177} = 0.042$$

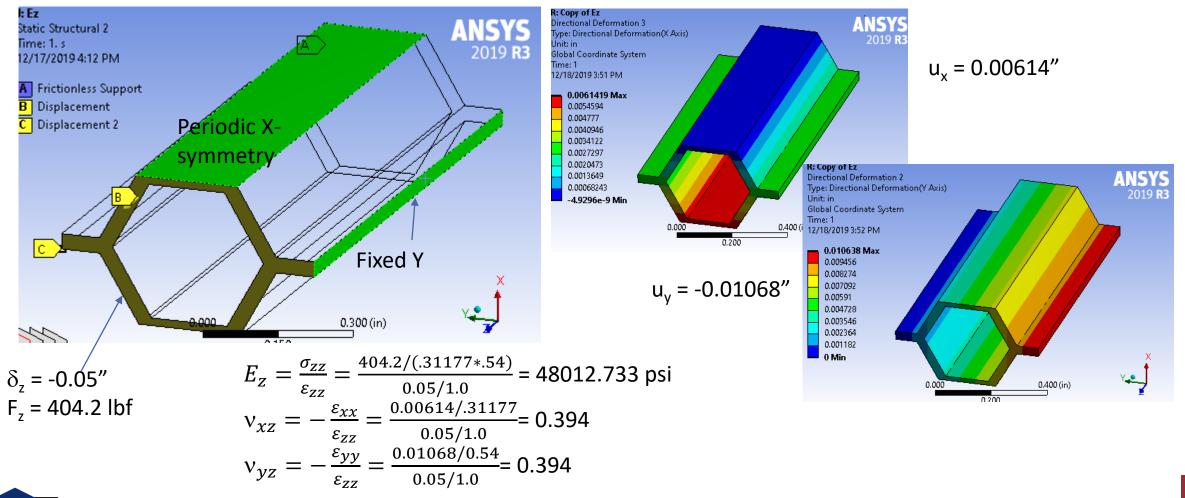
Even larger than the Material Designer estimate...!

Case 2: Uniaxial Tension (X-Z plane)



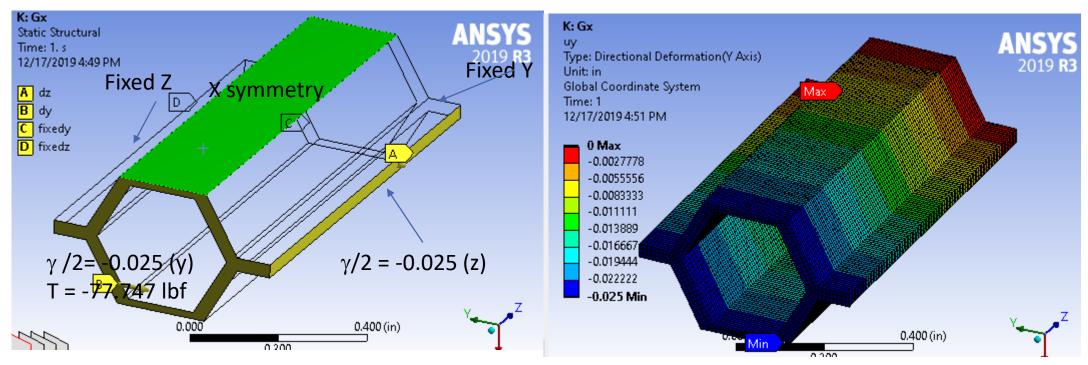


Case 3: Uniaxial Tension (X-Y plane)



Transverse deflections

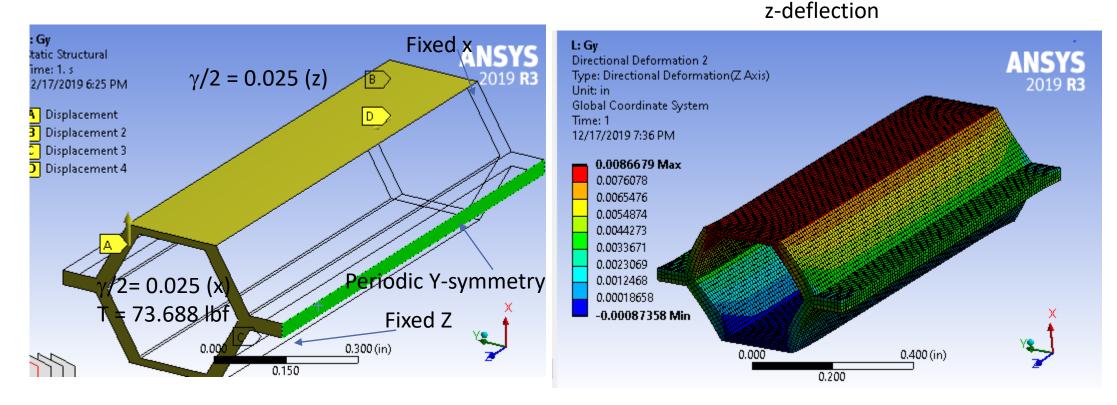
Case 4: Pure Shear (Y-Z plane)



$$G_{\chi} = \frac{\tau_{yz}}{\gamma_{yz}} = \frac{-\frac{-77.747}{0.54*.31177}}{0.05} = 9236.03 \text{ psi}$$



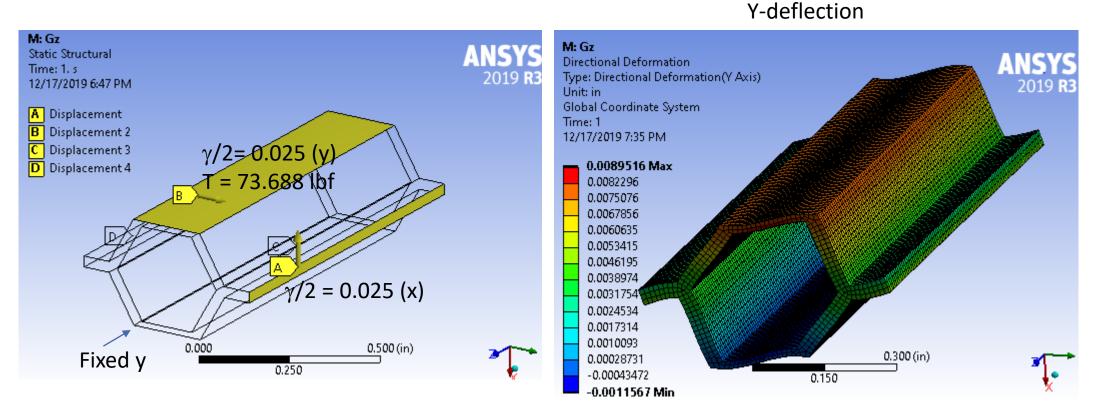
Case 5: Pure Shear (X-Z plane)



$$G_{\chi} = \frac{\tau_{yz}}{\gamma_{yz}} = \frac{-\frac{73.688}{0.54*.31177}}{0.05} = 8753.842 \text{ psi}$$



Model Validation: The "Old-Fashioned Way" (cont.) Case 6: Pure Shear (X-Y plane)



$$G_{\chi} = \frac{\tau_{yz}}{\gamma_{yz}} = \frac{-\frac{26.28}{0.54*1.0}}{0.050} = 973.550 \text{ psi}$$



Model Validation: Comparison

- Ok. Let's compare what we've got
- Off the bat, our immediate concern is the difference in Poisson ratios highlighted in light red
- After that, we see that the y-direction constants seem to show greater-than-average disagreement. Let's address both of these concerns
- We should remark that these sorts of discrepancies aren't unusual. Also, the Material Designer values are the more accurate ones (see the "Discussion" section at the end), but there ARE ways to get better accuracy from the Poisson ratios we've calculated the old-fashioned way!

Orhotropic Constan	t Material Designer	Old-Fashioned Way	Percent difference
Ex	3817.70	3692.20	-3.29
Ey	3817.60	3618.90	-5.20
Ez	48017.00	48012.70	-0.01
ν_{xy}	0.86	0.89	2.93
ν _{yz}	0.03	0.04	21.26
ν _{xz}	0.03	0.04	39.30
G _{xy}	996.85	973.60	-2.33
G _{yz}	9444.90	9236.03	-2.21
G _{xz}	9445.10	8753.80	-7.32



- First, we need to understand how the various constants are used in ANSYS. From the MAPDL Theory Reference (section 2.1.1. Stress-Strain Relationships)
- The Poisson ratios listed in Material Designer get implemented as the major (upper diagonal) Poisson ratios in MAPDL

$$\begin{bmatrix} D \end{bmatrix}^{-1} = \begin{bmatrix} 1/E_x & -v_{xy}/E_x & -v_{yz}/E_y & 0 & 0 & 0 \\ -v_{yx}/E_y & 1/E_y & -v_{yz}/E_y & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{xy} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{yz} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{xz} \end{bmatrix}$$
 Also, the $[D]^{-1}$ matrix is presumed to be symmetric, so that:

$$\begin{bmatrix} V_{yx}}{E_y} = \frac{v_{xy}}{E_x} \end{bmatrix}$$
 (2-5)
where typical terms are:

$$E_x = Young's modulus in the x direction (input as EX on MP command)$$

$$v_{xy} = major Poisson's ratio (input as PRXY on MP command)$$

$$v_{yx} = minor Poisson's ratio (input as RXY on MP command)$$

$$G_{xy} = shear modulus in the x y plane (input as GXY on MP command)$$

- We see from slide 24, that v_{xz} and v_{yz} seem to equal one another to three decimal places. And because these Poisson ratios should be more accurate than their transpose counterparts (because of the much greater stiffness in z, these values will be driven more by material –rather than geometric behavior), we can use these values to estimate the less accurate ratios calculated directly
- We should be careful here. The convention we have used to define v_{xz} and v_{yz} on slide 24 was adopted from that found on <u>https://en.wikipedia.org/wiki/Poisson%27s_ratio</u>. That is to say

$$\nu = -\frac{d\varepsilon_{\text{trans}}}{d\varepsilon_{\text{axial}}} \longrightarrow \text{Applied load is in axial direction}$$
$$\nu_{\chi Z} = -\frac{\varepsilon_{\chi \chi}}{\varepsilon_{\chi Z}}$$

- So that,
- However, according to the ANSYS convention, these are actually the major Poisson ratios! In other words, the smaller Poisson ratios we calculated in slides 22 and 23 (and reported in slide 28) should be minor Poisson ratios, while the larger ones calculated in slide 24 should be the major ones (this issue arises due to ambiguity over the ordering of the subscripts)! How do we know which should go where?

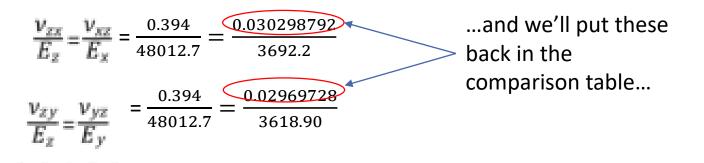
 \mathcal{E}_{ZZ}

- The answer is: Because of relations 2-5 thru 2-7, it doesn't matter! We just have to follow the convention used by Material Designer and stay consistent
- This is what we'll do to estimate better values for the Poisson ratios...

• But before we do, let's see why we CAN'T just use the more accurate Poisson ratios, $v_{xz} = v_{yz}$ = 0.394, and report those as major Poisson ratios. If we did that, following relation 2-6 and 2-7, we would have the following:

$$\frac{v_{zx}}{E_z} = \frac{v_{xz}}{E_x} = \frac{0.394}{3692.2} = \frac{5.12}{48012.7}$$
 This is out of bounds...!

- A similar problem arises for v_{yz} . Relations 2-5 thru 2-7 thus force us to conclude that the larger Poisson ratios MUST be minor Poisson ratios. Another (perhaps far simpler) way to remember this is to note that, in the corresponding terms in the flexibility matrix, D⁻¹, the denominators always correspond to the applied load (!)
- We can then use these to calculate the major Poisson ratios as follows:





- Let's update our comparison table with the adjusted values
- This new comparison is about as good as we could hope for

	Orhotropic Constant	Material Designer	Old-Fashioned Way	Percent difference	-
_	Ex	3817.70	3692.20	-3.29	
	Ey	3817.60	3618.90	-5.20	adjusted values
_	Ez	48017.00	48012.70	-0.01	to within 2 decimal places
_	ν _{xy}	0.86	0.89	2.93	procee
	$\nu_{\gamma z}$	0.03	0.03	-2.67	
	ν _{xz}	0.03	0.03	0.49	
_	G _{xy}	996.85	973.60	-2.33	
_	G _{yz}	9444.90	9236.03	-2.21	
_	G _{xz}	9445.10	8753.80	-7.32	



Model Validation: Actual vs. Homogenized

- And now for the real test
- We'll construct a part consisting of a 6 x 10 repeated pattern of our unit cell

Engineering Diata

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- Well fix it at one edge, and place a remote load at one edge of the structure's bounding box
- The idea is to apply a single load which incorporates some bending and twist, and compare the resultant displacement with a simple block model, which has no honeycomb structure, but DOES utilize the material properties we calculated with Material Designer.

2 🥏 Engineering Data

Engineering Data

Engineering Data

homogenized

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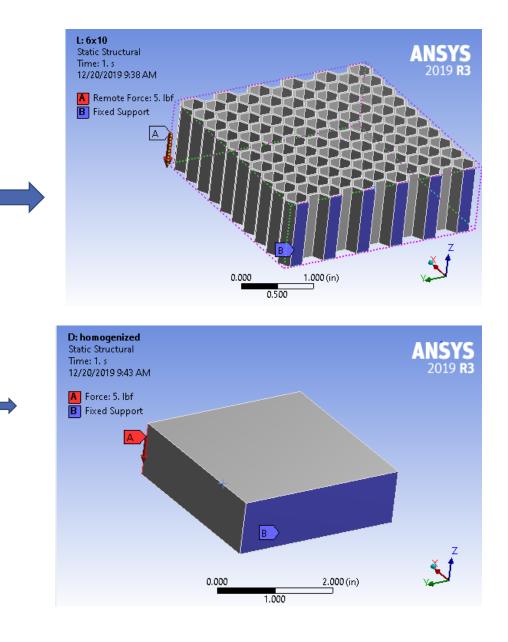
Geometr

Model

Setup

Solution

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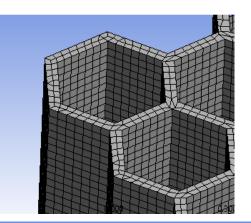


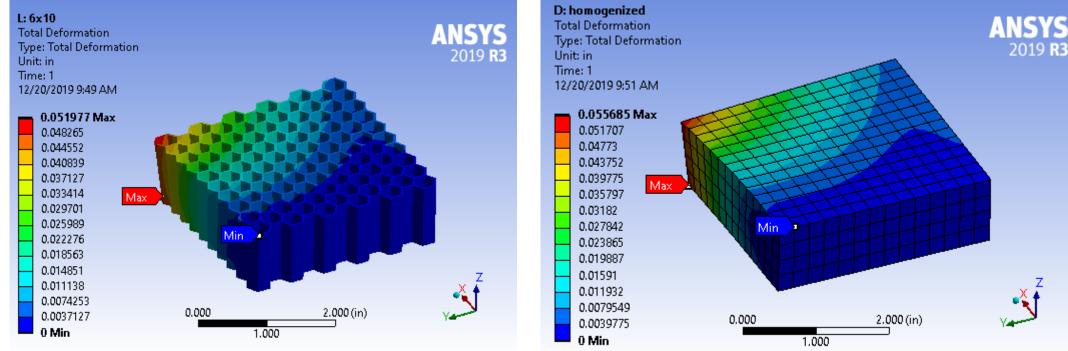
Model Validation: Actual vs. Homogenized

• The results look pretty good. They get better as we refine the honeycomb model (but we'll stop here, with 213,000 elements)

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Model Validation: Material Symmetry

- We promised (slide 13) that we would return to the question of material symmetry raised by Material Designer (under Analysis Settings).
- When no additional symmetry is chosen, orthotropic properties are assumed (reflection symmetry about the three global coordinate axes)
- Checking one of the three planes tells Material Modeler that there is additional rotational symmetry in that plane

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Model Validation: Material Symmetry (cont.)

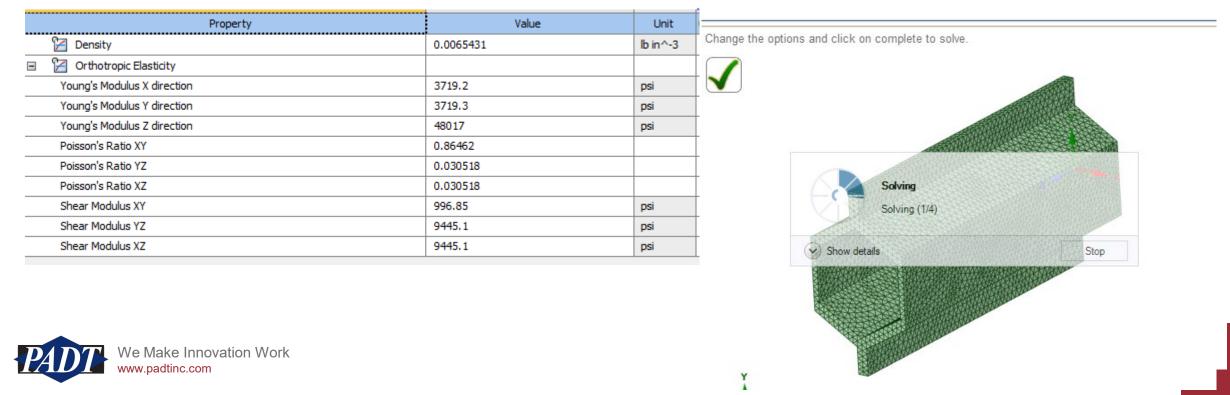
- Checking one of the planes under the additional symmetry options means that the material will be transversely isotropic in that plane
- Checking two or more will result in full isotropy
- The nearly identical values of Ex and Ey imply that the XY plane is isotropic, with a different modulus along the z-axis.
- We can test this by going back and checking the box which says "Use Material Symmetry in XY", and re-running the analysis

Property	Value	l	Jnit	
🔁 Density	0.0065431	lb ir	n^-3	
Orthotropic Elasticity				
Young's Modulus X direction	3718.7	psi		
Young's Modulus Y direction		3718.6	psi	
Young's Modulus Z direction	48017		psi	
Poisson's Ratio XY		0.86466		
Poisson's Ratio YZ		0.030513		
Poisson's Ratio XZ	0.030514			
Shear Modulus XY		996.85		
Shear Modulus YZ		9444.9	psi	
Shear Modulus XZ		9445.1	psi	



Model Validation Material Symmetry (cont.)

- When we do this, note that Material Designer now has to solve only 4 equations (instead of six)
- The result below pretty much confirms our observation (our results didn't change much). The extruded honeycomb structure is indeed transversely isotropic in the plane of the honeycomb
- If we had another isotropic plane (we don't), we could check that one as well, resulting in only two equations to solve, and so on...



Discussion

- The homogenized material properties calculated by Material Designer "should" produce more accurate values than what we've been calling "the old-fashioned way"
- The latter method simulates uniaxial tension/compression and torsion tests on a Unit Cell (UC) of a repeated structure. Under this assumption, the unit cell geometry is somewhat critical to obtaining good results. Also, the boundary conditions are unambiguous and always simulate the same type of material test(s)
- The theoretical principles behind the former method (what Material Designer does) are far more sophisticated. They are meant to more intimately relate a given RVE (which may or may not represent a repeated structure's UC) to the macro environment it is supposed to characterize (see the References section of Material Designer's documentation. But also see here:

https://deepblue.lib.umich.edu/bitstream/handle/2027.42/47812/466 2004 Article BF00369853.pdf?sequence=1&isAllowed=y

• The results are not critically reliant on the RVE geometry representing a true UC of a repeated structure



Conclusions

- This article summarizes the usage of ANSYS' new Material Designer tool
- The article also reviews the results of a simple case study and compares them to results obtained by more traditional means
- It is concluded that Material Designer offers an efficient, accurate, and comprehensive workflow for characterizing effective elastic properties.

