WINTER THESIS

DETERMINATION OF EFFECTIVE YOUNG'S MODULUS FOR RVES

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1. INTRODUCTION

Among the ever-growing problems faced by industries today, the requirement of lightweight and at the same time stiff structures has been a primary concern. To serve these requirements the development of composite materials has been crucial. Composite materials are those materials which are formed or fabricated using two or materials and the product of the process gives us a new material that has properties superior to that of the individual constituents. Therefore, one can say that composite materials are highly tailorable materials. In the process of bringing different materials together to form the product, the individual constituents retain their identity.

The two main components of a composite material are the matrix and the reinforcement. Matrix is of different types based on their compositions such as metal matrix, polymer matrix etc. Similarly, the reinforcements can be of different types such as metals, polymer fibers, ceramics etc. The different distribution of the reinforcement within the matrix or also known as the primary phase, results in different effective properties. The reinforcements can be randomly distributed and oriented or distributed and oriented in an ordered fashion. Different configurations of the fibers or reinforcements give us different properties for the material and hence there could be certain uncertainties at different scales. The properties of such tailored materials also depend on the type of manufacturing process adopted.

The enhanced and improved properties of composite materials make them an ideal replacement for metals in certain structures. Properties such as high specific strength, high flexibility, excellent thermal and mechanical durability, high surface hardness etc. have drawn manufacturers into using composite materials in their designs. The desire and requirement to incorporate such materials have boomed and therefore in depth analysis has to be carried out to make the material more efficient so as to serve its purpose and also to understand the existing uncertainties at the varying scales. Among the different analysis and tests the homogenization and determination of effective mechanical properties gives a holistic view onto the capabilities of the formed material. By homogenizing the elastic stiffness properties between scales, effective elastic properties of the material can be derived. Experimental methods to determine the effective mechanical properties has the disadvantages of resource requirements, time consumption, intense labour requirements etc. Another approach to determine the properties is to use semi-analytical methods that involves a lot of assumptions. Due to the use of assumptions the obtained results are not accurate, and accuracy falls when composites with complex micro-structures are analyzed. Hence a numerical approach towards the homogenization and determination of effective properties can come in handy since the time, resource requirements are comparatively minimal, and the results are far more reliable than the ones from the semi analytical approach. Among the different homogenization techniques such as the Chamis micromechanical model equations, asymptotic mean-field homogenization technique etc. (which are theoretical formulations), there exists an incapability to consider the geometric complexities and variation in materials at the microscale level. An efficient numerical approach to obtaining effective properties by homogenization is the finite element-based approach using a representative volume element i.e. RVE. This approach is becoming popular due to its capability to accurately predict the effective mechanical properties of a composite material, ease of implementation and its capability to consider the complex microstructure of the composite material. To find the effective properties of a composite material through numerical methods, the whole structure need not be taken into account. Instead, a small volume element of the structure is enough to be used as the model to derive the effective properties of the entire structure.

1.1 RVEs and Periodic boundary conditions

Representative volume element or RVE, is defined as a smallest material volume element of the material that can be used as a model to represent mean constitutive responses. The selection of the RVE would be based on whether when it is duplicated multiple times and brought together, the formed section represents the larger scale of the material. The RVE modeled for a structure must include an adequate number of microstructural features to ensure that the boundary conditions applied at the composite surface do not influence its overall effective properties. Hence it could be said that a modeled RVE must contain a large sufficient volume that will contain the sufficient features of the original scale. The overall effective properties of the structure can be obtained by averaging the stress, strain or energy fields derived from the analysis of its RVE. While modeling an RVE capturing the sufficient volume of microstructure of the original structure is important and at the same time the RVE must be geometrically periodic as well as it should be periodic across the edges, corners and its faces. For any fiber or reinforcement that is not wholly included within the model, its remaining should be included within the RVE to justify and validate its periodicity. RVE with a single fiber tend to show much variation in results when compared to the experimental results. In literature it has been pointed out that this behavior is due to absence of shielding effect provided by the neighboring fibers as they are not included within the volume considered.

Homogenization using RVE considers the boundaries of the volume element as well since these boundaries share the region with the rest of the structure. Therefore, while considering these boundaries necessary boundary conditions should also be considered. The selection of the right boundary conditions for the RVE has always been a problem for this homogenization approach. The boundary conditions should be chosen such that they satisfy Hill's energy law. This energy law states that the energy on the microlevel should be equal to the effective energy of the composite material that is homogenized. Uniform tensile boundary condition, linear displacement boundary condition and periodic boundary condition are those which satisfy the Hill's energy law criteria. From literature it is understood that both uniform tensile boundary condition and linear displacement boundary condition does not provide accurate and reliable results for effective properties when compared to periodic boundary conditions (PBCs). Use of PBCs helps in mimicking the behavior of the larger structure by the small volume element RVE. Applying PBCs ensures that the deformation of external surfaces remains periodic.When PBCs are applied, the numerical analysis converges quickly and accurately. The speed to converge increases as the RVE size is increased. With the help of Lagrange multiple method, PBCs can be easily set up for periodic RVEs. Another way of applying PBCs on a RVE is by using constraint eliminations. By this periodic behavior can be achieved by linking the nodal degrees of freedom of the FE model. Having a periodic RVE helps in applying periodic meshes as well. Applying a periodic mesh shall implies that there exists the same mesh distribution on two opposite faces of the RVE. For efficient application of periodic boundary condition, periodic meshes are essential. Though not accurate for non-periodic meshes, a weak enforcement of PBC using the Lagrange multiple over the point-to-point enforcement results in a less stable result. There are studies mentioned in the literature that consider cases where the meshes are not periodic. Here they use a master/slave approach for applying periodic boundary conditions on the non-periodic meshes or sites. Another method mentioned in the literature is the use of Lagrange shape functions to arrive at a displacement field at the intersection of fibers with the RVE sides when an arbitrary non periodic mesh is encountered. This method when considered for the entire RVE will work to impose the PBCs without the need for a periodic mesh.

The work carried out involves the estimation of effective elastic properties of a composite material made using Polypropylene and E-glass fibers with the help of a single fiber RVE, unidirectional multi-fiber RVE and bidirectional multi-fiber RVE using ABAQUS ver.2023. In the analysis, periodic boundary conditions are not used.

2. METHODOLOGY

2.1 Materials properties

Matrix: Polypropylene

PROPERTY	
Young's Modulus	1.308 GPa
Poisson's ratio	0.40
Yield strength	40 Mpa
Volume fraction	40%

Fiber: E-glass

PROPERTY	
Young’s Modulus	73 GPa
Poisson’s ratio	0.2
Volume fraction	60%

2.2 Geometry

The following are the RVE dimensions

Length	100 um
Width	100 um
Height	100 um

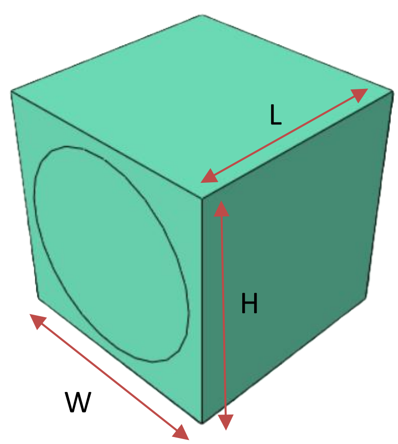


Fig. Dimensions of RVE

The diameter of the fibers was estimated from the fiber volume fraction (V_f) formula.

$$Vf = \frac{N\pi D_f^2}{4HW}$$

$$\rightarrow \qquad D_f^2 = \frac{4HW}{N\pi}$$

Where D_f :diameter of the fiber

H : height of RVE

W : width of RVE

N : number of fibers

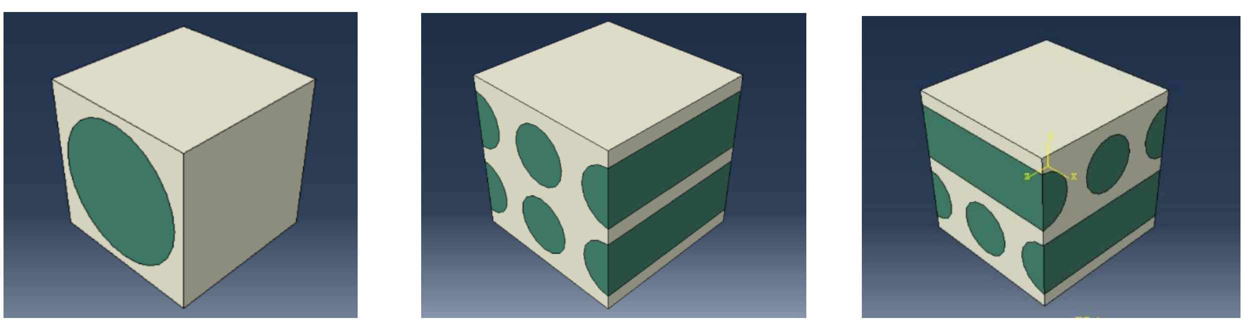
V_f: volume fraction of fiber

For a single RVE i.e. N=1

D_f=87.40 um

For multiple fibers say N=6

D_f=35.68 um



(a) (b) (c)

Fig. Modelled RVE's with (a) single fiber, (b) unidirectional multiple fibers and (c) bidirectional multiple fibers

- For single fiber RVE

Once the model was created in the PART interface of ABAQUS, it assembeled and material properties of E-glass were applied to the fiber while the material properties of Polypropylene were applied for the matrix. After assembling the model it is meshed with a mesh size of 5. The boundary conditions and constraints varied with respect to the type of load. The loading cases that were carried out included X tension, Y tension, Z tension, XY shear, XZ shear, YZ shear. Rather than applying the load to the face of the RVE two reference points were used to load the RVE by constraining the reference point to the face onto which the load was supposed to act on.

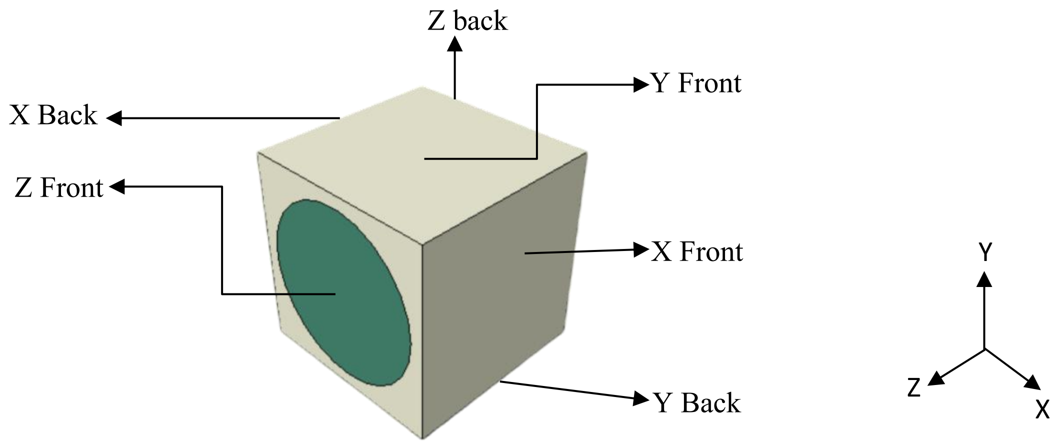


Fig. Different faces of the RVE

The following are the loads and boundary conditions applied for the different loading cases:

1. X tension

Load: tensile displacement load of 12 um in X directions

Boundary conditions: roller in X, Y and Z back face of the RVE

2.Y tension

Load: tensile displacement load of 12 um in Y direction

Boundary conditions: roller in X, Y and Z back face of the RVE

3.Z tension

Load: tensile displacement load of 12 um in Z direction

Boundary conditions: roller in X, Y and Z back face of the RVE

4.XY shear

Load: Shear force of 10 um in Y direction in X plane

Boundary conditions: Back face of Y fixed in Z and X direction

Back face of X fixed in Y and Z direction

5.XZ shear

Load: Shear force of 10 um in Z direction in X plane

Boundary conditions: Back face of X fixed in Z and Y direction

Back face of Z fixed in X and Y direction

6.YZ shear

Load: Shear force of 10 um in Z direction in Y plane

Boundary conditions: Back face of Y fixed in Z and X direction

Back face of Z fixed in X and Y direction

- For multiple fiber RVE

Once the model was drafted in the ABAQUS Part interface, it was assembled and material properties for fiber and matrix were applied. For the unidirectional RVE, 'hex' mesh of size 5 was used while for the bidirectional RVE 'tet' type mesh of size 10 was used. Once the models were meshed the load and boundary conditions were applied. Similar to the single fiber RVE, a reference point was used to load the model. Loading was achieved by constraining the reference point and the face on which the load should be applied.

The following were the loading cases:

1. X tension

Load: tensile displacement load of 10 um in X directions

Boundary conditions: roller in X, Y and Z back face of the RVE

2.Y tensile

Load: tensile displacement load of 10 um in Y direction

Boundary conditions: roller in X, Y and Z back face of the RVE

3.Z tensile

Load: tensile displacement load of 10 um in Z direction

Boundary conditions: roller in X, Y and Z back face of the RVE

4.XY shear

Load: Shear force in Y direction in X plane

Boundary conditions: Front face of X fixed in X direction

Back face of X fixed in X, Y, Z direction

5. XZ shear

Load: Shear force in X direction in Z plane

Boundary conditions: Front face of Z fixed in Z direction

Back face of Z fixed in X, Y, Z direction

6.YZ shear

Load: Shear force in Z direction in Y plane

Boundary conditions: Back face of Y fixed in X, Y, Z direction

Front face of Y fixed in Y direction

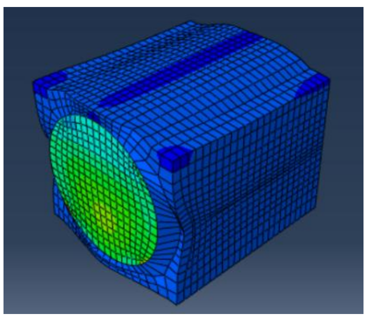
3. RESULTS

The average values of stress and strain obtained through the analysis corresponds to the stress and strain of the material at larger scales. Since the structure in hand is homogenized with the help of an RVE, the overall effective elastic properties can be evaluated by averaging the stress and strain values obtained by the postprocessing of the analysis data of the RVE under varying loading conditions.

3.1. For single fiber RVE

The following are the Young's modulus results obtained after the averaging process:

Loading Case	Young's modulus E (GPa)
X tensile force	8.342
Y tensile force	8.313
Z tensile force	36.561
XY shear force	3.077
YZ shear force	3.829
XZ shear force	5.814



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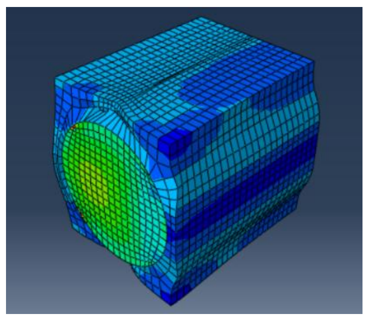

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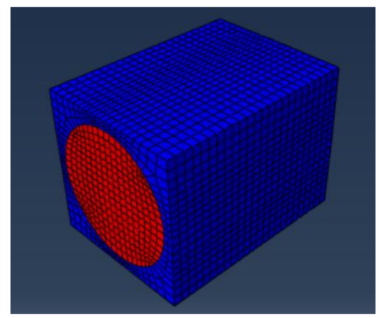

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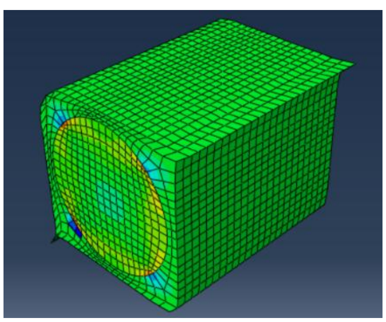

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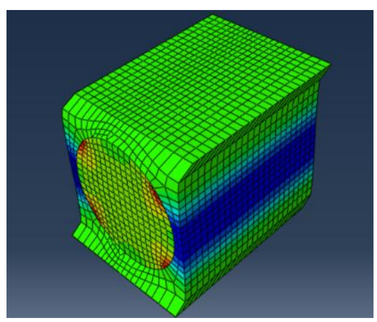

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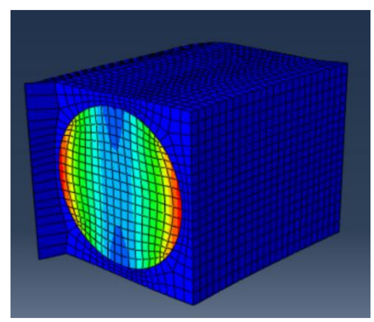


(f)

Fig. (a), (b), (c) are the deformation and stress hotspots of single fiber RVE models subjected to tensile force in X, Y, Z directions respectively. (d), (e), (f) are the deformations and stress hotspots of models subjected to shear forces.

3.2. For unidirectional multi-fiber RVE

The following are the Young's modulus results obtained after the averaging process:

Loading Case	Young's modulus E (GPa)
X tensile force	4.479
Y tensile force	4.406
Z tensile force	24.370
XY shear force	0.755
YZ shear force	1.808
XZ shear force	1.243

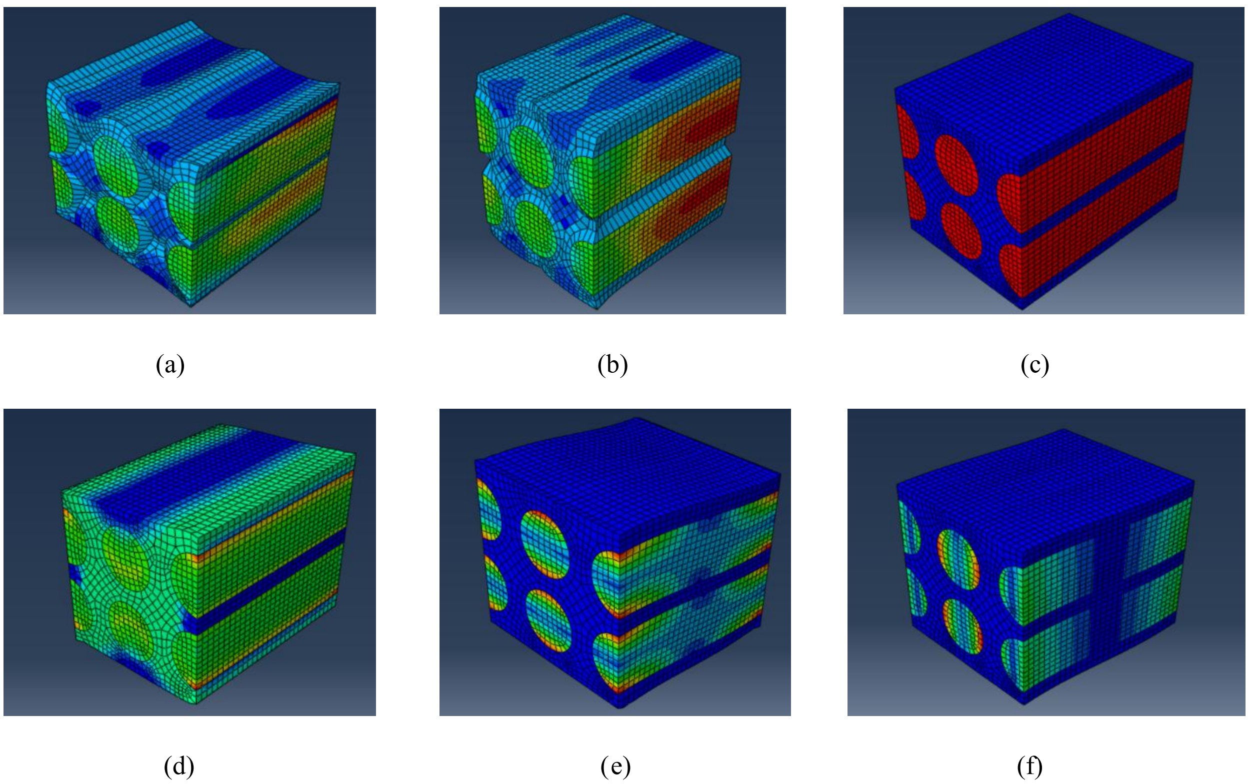
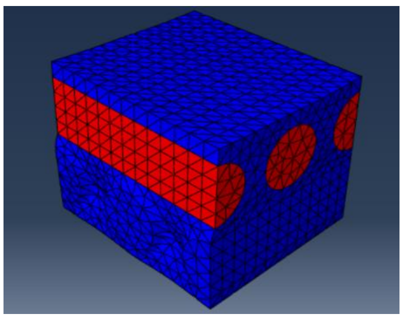


Fig. (a), (b), (c) are the deformation and stress hotspots of unidirectional RVE models subjected to tensile force in X, Y, Z direction respectively. (d), (e), (f) are the deformations and stress hotspots of models subjected to shear forces

3.3. For bi-directional multi-fiber RVE

The following are the Young's modulus results obtained after the averaging process:

Loading Case	Young's modulus E (GPa)
X tensile force	16.070
Y tensile force	2.223
Z tensile force	16.051
XY shear force	1.693
YZ shear force	0.637
XZ shear force	1.149



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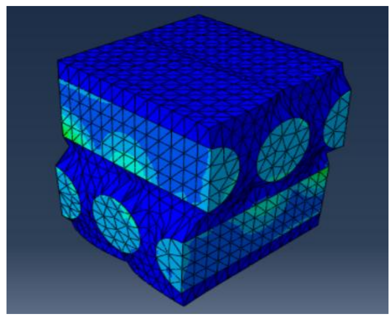

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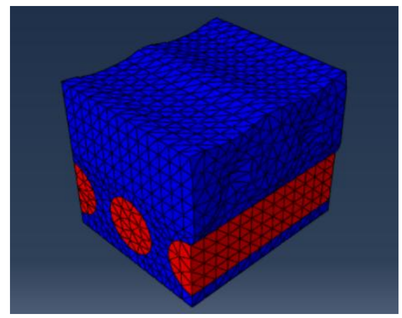

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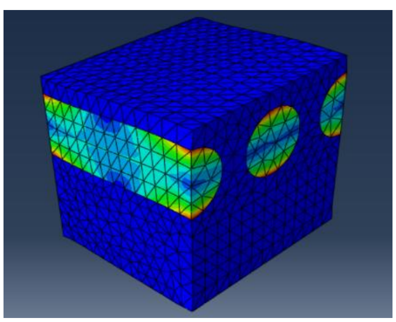

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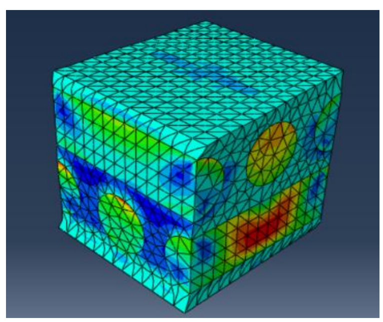
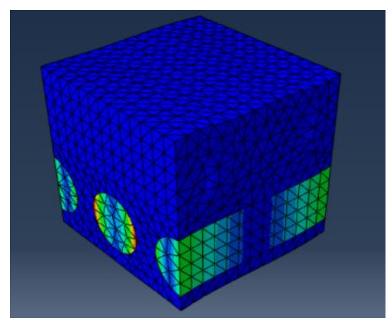


(e)



(f)

Fig. (a), (b), (c) are the deformation and stress hotspots of bidirectional RVE models subjected to tensile force in X, Y, Z direction respectively. (d), (e), (f) are the deformations and stress hotspots of models subjected to shear forces

From the results obtained it is evident that the predicted Young's modulus of the models is highest in the direction along which the fibers are laid. For the single fiber RVE, the Young's modulus is highest for the case where it is loaded in the Z direction. In the case of the bidirectional RVEs, it is seen that the Young's modulus along both X and Z direction are relatively the same and stands high when compared to the Young's modulus obtained by loading the bidirectional modal in the

Y direction. When it comes to the shear loading cases the models exhibit lesser elastic property when compared to cases where it was loaded with tensile loads.

REFERENCES

1. V.D. Nguyen, E. Bechet, C, Geuzaine, L Noels, Imposing periodic boundary condition on arbitrary meshes by polynomial interpolation. https://doi:10.1016/j.commatsci.2011.10.017
2. Sunday C. Aduloju, Timothy J. Truster, A primal formulation for imposing periodic boundary conditions on conforming and nonconforming meshes. https://doi.org/10.1016/j.cma.2019.112663
3. Sadik L. Omairey, Peter D. Dunning, Srinivas Sriramula, Development of an ABAQUS plugin tool for periodic RVE homogenization https://doi.org/10.1007/s00366-018-0616-4
4. Wenlong Tian, Lehua Qi, Xujiang Chao, Junhao Liang, Mingwang Fu, Periodic boundary condition and its numerical implementation algorithm for evaluation of effective mechanical properties of the composites with complicated micro-structures https://doi.org/10.1016/j.compositesb.2018.10.053
5. https://www.youtube.com/watch?v=d28xZTQapcQ