

PREDICTION OF COMPOSITE PROPERTIES FROM A REPRESENTATIVE VOLUME ELEMENT

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Abstract

A vigorous mechanics foundation is established for using a representative volume element (RVE) to predict the mechanical properties of unidirectional fiber composites. The effective elastic moduli of the composite are determined by finite element analysis of the RVE. It is paramount in such analyses that the correct boundary conditions be imposed such that they simulate the actual deformation within the composite; this has not always been done previously. In the present analysis, the appropriate boundary conditions on the RVE for various loading conditions are determined by judicious use of symmetry and periodicity conditions. The non-homogeneous stress and strain fields within the RVE are related to the average stresses and strains by using Gauss theorem and strain energy equivalence principles. The elastic constants predicted by the finite element analysis agree well with existing theoretical predictions and available experimental data.

Keywords: elastic moduli, micromechanics, representative volume element, unit cell, boundary conditions

1 INTRODUCTION

Prediction of the mechanical properties of a unidirectional fiber-reinforced composite has been an active research area for the past two decades. Several theoretical models have been proposed for the prediction of composite properties from those of the constituent fiber and matrix. In particular, upper and lower bounds for composite elastic moduli have been derived¹ using energy variational principles, and closed-form analytical expressions have been obtained.² A survey of the existing micromechanical models has been carried out.³ Among the elastic constants predicted by these models, the longitudinal modulus and Poisson's ratio show good agreement with experiments and can be approximated by the simple rule of mixtures. The predictions for the other elastic constants, however, show significant scatter and

depend upon the assumed geometrical model of the composite. Experimental determination of the unidirectional composite moduli is difficult, especially when it involves determining the longitudinal and transverse shear moduli. Thus, numerical techniques like finite element methods are needed to verify the feasibility of the models.

Numerical methods to estimate composite properties usually involve analysis of a representative volume element (RVE) corresponding to a periodic fiber packing sequence. Several papers exist in the literature where the RVE is analysed to determine composite moduli. There are a few issues that need to be carefully considered when carrying out such analyses.

Firstly, the correct RVE corresponding to the assumed fiber distribution must be isolated. This has not always been done correctly. For example, Shi *et al.*⁴ modeled a hexagonal (staggered) distribution of short fibers by a RVE that actually represents a square array fiber distribution.

Secondly, correct boundary conditions need to be applied to the chosen RVE to model different loading situations. Proper consideration must be given to the periodicity and symmetry of the model in arriving at the correct boundary conditions. Under longitudinal and transverse normal loading, a typical RVE can deform in such a way that it remains a right parallelepiped, i.e. plane sections remain plane. This has been correctly modeled by several researchers.^{5–8} However, when it comes to modeling longitudinal and transverse shear loading, many researchers have made incorrect assumptions about the deformed shape of the RVE. Naik⁷ and Brockenbrough *et al.*⁸ modeled transverse shear loading assuming that the deformed boundary of the RVE remained plane (no distortion). Caruso⁹ also made a similar assumption about the deformed shape under transverse shear loading and noted that 'the finite element predictions for G_{23} are not very reliable in view of the difficulty associated with simulating the respective boundary conditions'. The present research revealed that the assumptions made by these researchers are not true, i.e. the

boundaries of the RVE under transverse shear loading can distort while still exhibiting a periodic displacement field. Zhang and Evans¹⁰ modeled longitudinal shear loading in a composite cylinder model assuming a constant shear strain for both the fiber and the matrix. This assumption is incorrect, since the fiber and matrix with different elastic moduli should have different shear strains. Adams and Crane¹¹ used the correct boundary conditions to model longitudinal shear loading. In order to do so, however, they had to develop their own two-dimensional finite element model with a special strain-displacement relationship.

Another important issue that has not been addressed in any of the literature reviewed is the relationship between the actual non-homogeneous stress and strain fields within the RVE and the 'average' stress and strain for the composite. The relationship between the two and the procedure for determining the 'average' quantities are discussed here.

In the present paper, the procedure for predicting the elastic constants of the composite from the RVE is laid on a rigorous mechanics foundation by using strain energy equivalence principles in conjunction with three-dimensional finite element analysis. The method works as follows. First, the appropriate boundary conditions for a typical RVE under different loading are determined and applied to the finite element model. The non-homogeneous strain fields obtained from the analysis are reduced to a volume-averaged strain by using Gauss theorem to integrate the surface displacements. The average stress is then determined by using the strain energy equivalence principle to relate the energy stored in the RVE to the external work done on it. The relevant composite modulus is then obtained as the ratio of the average stress to the average strain.

The elastic constants obtained from the analysis are compared with predictions of several micromechanical theories and with available experimental data. This procedure can also be extended to describe non-linear response of composites by modeling the matrix as an elastic-plastic material.

2 REPRESENTATIVE VOLUME ELEMENT (RVE)

In a composite lamina the actual fiber distribution is quite random across the cross-section. For simplicity reasons, most micromechanical models assume a periodic arrangement of fibers for which a RVE or unit cell can be isolated. The RVE has the same elastic constants and fiber volume fraction as the composite. The periodic fiber sequences commonly used are the square array and the hexagonal array. The corresponding RVE are shown in Fig. 1.

When modeling composites using a RVE it is important to look closely at how it deforms when a uniform tensile or shear load is applied at the boundary of the composite. In a homogeneous material a uniform stress and strain state will exist under uniform loading, but such is not the case in a composite which is composed of fibers and matrix with vastly different properties. However, since all the RVEs are identical, they should exhibit identical stress and strain fields. Thus, from a global perspective, the stress and strain fields will be periodic in nature, except in a narrow boundary layer where the external load is applied. These periodicity constraints are used to determine the appropriate displacement constraints at the boundary of the RVE.

In classical lamination theory the composite lamina is modeled as a homogeneous orthotropic medium with certain effective moduli that describe the 'average' material properties of the composite. To describe this macroscopically homogeneous medium, macro-stress and macro-strain are derived by averaging the stress and strain tensor over the volume of the RVE:

$$\bar{\sigma}_{ij} = \frac{1}{V} \int_V \sigma_{ij}(x, y, z) dV \quad (1)$$

and

$$\bar{\epsilon}_{ij} = \frac{1}{V} \int_V \epsilon_{ij}(x, y, z) dV \quad (2)$$

The equivalence between the actual heterogeneous composite medium and the homogeneous medium

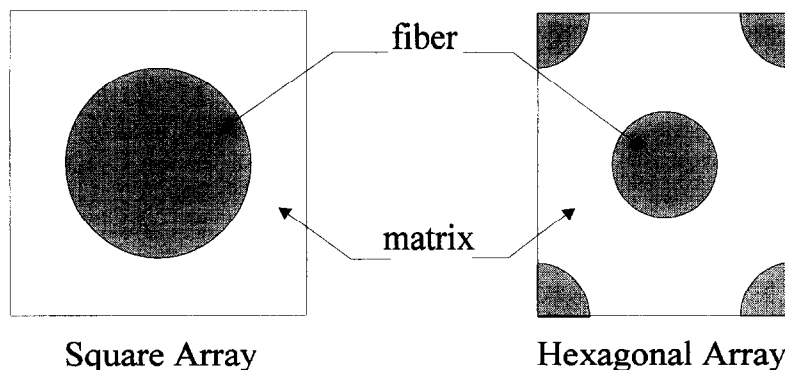


Fig. 1. RVE for square and hexagonal array configurations.

given by the average stresses and strains and the effective elastic constants needs to be reviewed. For this purpose we subject the RVE to appropriate boundary tractions t_i or boundary displacements u_i that would produce uniform stresses ($\bar{\sigma}_{ij}$) and strain ($\bar{\epsilon}_{ij}$) in a homogeneous medium.

The total strain energy U stored in the a volume V of the effective medium is:

$$U = \frac{1}{2} \bar{\sigma}_{ij} \bar{\epsilon}_{ij} V \quad (3)$$

The strain energy U' stored in the heterogeneous RVE of volume V is:

$$U' = \frac{1}{2} \int_V \sigma_{ij} \epsilon_{ij} dV \quad (4)$$

$$= \frac{1}{2} \int_V \sigma_{ij} (\epsilon_{ij} - \bar{\epsilon}_{ij} + \bar{\epsilon}_{ij}) dV \quad (5)$$

$$= \frac{1}{2} \int_V \sigma_{ij} (\epsilon_{ij} - \bar{\epsilon}_{ij}) dV + \frac{1}{2} \bar{\epsilon}_{ij} \int_V \sigma_{ij} dV \quad (6)$$

$$= \frac{1}{2} \int_V \sigma_{ij} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial \bar{u}_i}{\partial x_j} \right) dV + \frac{1}{2} \bar{\sigma}_{ij} \bar{\epsilon}_{ij} V \quad (7)$$

Subtracting eqn (3) from eqn (7) yields:

$$U' - U = \frac{1}{2} \int_V \sigma_{ij} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial \bar{u}_i}{\partial x_j} \right) dV \quad (8)$$

Using the equilibrium equation:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \quad (9)$$

we can write eqn (8) as:

$$U' - U = \frac{1}{2} \int_V \frac{\partial}{\partial x_j} [\sigma_{ij} (u_i - \bar{u}_i)] dV \quad (10)$$

The volume integral in eqn (10) can be converted into a surface integral by using Gauss theorem. Thus:

$$U' - U = \frac{1}{2} \int_S \sigma_{ij} (u_i - \bar{u}_i) n_j dS \quad (11)$$

where S is the surface and n the unit outward normal. On the surface S :

$$u_i = \bar{u}_i \quad (12)$$

Thus:

$$U' - U = 0 \quad (13)$$

The average stress and strain quantities defined in

eqns (1) and (2) thus ensure equivalence in strain energy between the equivalent homogeneous material and the original heterogeneous material. These average quantities will be used in the subsequent analysis to determine composite moduli.

3 DETERMINATION OF AVERAGE STRAIN FROM BOUNDARY DISPLACEMENTS

The finite element analysis of the RVE yields the stress and strain fields within the heterogeneous material. The corresponding average quantities (i.e. $\bar{\sigma}_{ij}$ and $\bar{\epsilon}_{ij}$) can be obtained by taking a volume average using eqns (1) and (2). This can be a cumbersome task, especially if a large number of elements is used. Alternatively, the average strain can be related to the boundary displacements of the RVE by using Gauss theorem, where eqn (2) becomes:

$$\bar{\epsilon}_{ij} = \frac{1}{V} \int_V \epsilon_{ij} dV = \frac{1}{2V} \int_S (u_i n_j + u_j n_i) dS \quad (14)$$

where V is the volume of the RVE, S is the boundary surface of the RVE, u_i is the i th component of displacement and n_j is the j th component of the unit normal to S .

Strictly speaking, eqn (14) is valid only when ϵ_{ij} is continuous in V . In the present analysis, ϵ_{ij} is only piecewise continuous as there exists a strain discontinuity at the fiber/matrix interface and we need to show that Gauss theorem is still valid under such circumstances.

Consider the unit cell for the square array shown in Fig. 2. We can apply a cut as shown and make the matrix a simply connected region. Gauss theorem can be applied within the individual fiber and matrix phases since the strains are continuous within them. The average strain can be calculated as:

$$\begin{aligned} \bar{\epsilon}_{ij} &= \frac{1}{V} \left(\int_V \epsilon_{ij} dV \right) \\ &= \frac{1}{V} \left(\int_{V_f} \epsilon_{ij} dV + \int_{V_m} \epsilon_{ij} dV \right) \\ &= \frac{1}{V} \left(\underbrace{\frac{1}{2} \int_{S_1} (u_i n_j + u_j n_i) dS}_{\text{fiber}} \right. \\ &\quad \left. + \underbrace{\frac{1}{2} \int_{S_2} (u_i n_j + u_j n_i) dS - \frac{1}{2} \int_{S_1} (u_i n_j + u_j n_i) dS}_{\text{matrix}} \right) \quad (15) \end{aligned}$$

At the interface the displacements are continuous since there is assumed to be perfect bonding between the fiber and the matrix. Thus the first and third integrals in eqn (15) cancel each other and we are left

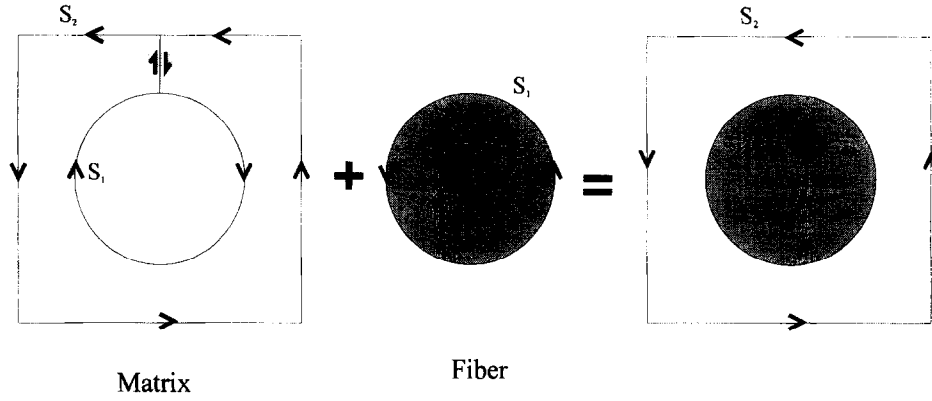


Fig. 2. Integration contour for square array.

to deal with only the displacements at the boundary of the unit cell. Thus:

$$\bar{\epsilon}_{ij} = \frac{1}{V} \int_{S_2} (u_i n_j + u_j n_i) dS \quad (16)$$

where S_2 denotes the outer boundary of the unit cell. In a similar manner, the same relationship can be derived for a hexagonal array by integrating along the cuts shown in Fig. 3. The relationship given by eqn (16) makes it possible to evaluate the volume averaged strains using the boundary displacements, thus avoiding the volume integration.

4 FINITE ELEMENT MODELING

4.1 Normal loading

The RVE used in the analysis to model normal loads is shown in Fig. 4. Only a quadrant of the original RVE (Fig. 1) is modeled since there are two axes of symmetry in this problem. The cross-section of the square array model (Fig. 4) in the y - z plane is a square ($b = c$), while that of the hexagonal array model is a rectangle ($b = c/\sqrt{3}$). The length a along the fiber axis for both models is chosen to be equal to b .

Axial loading is modeled by a force P_1 acting on the face $x = a$, while transverse loading corresponds to a force P_i acting on the face $y = b$ or $z = c$. For such loading conditions, the boundaries of the RVE also correspond to lines of symmetry. Thus, normal displacements of the boundaries of the quadrant are restricted to those that cause the boundary to displace only parallel to the original boundary. The displacement constraints applied to the finite element model are:

$$\begin{aligned} u(0, y, z) &= 0 \\ u(a, y, z) &= \text{constant} = \delta_1 \\ v(x, 0, z) &= 0 \\ v(x, b, z) &= \text{constant} = \delta_2 \\ w(x, y, 0) &= 0 \\ w(x, y, c) &= \text{constant} = \delta_3 \end{aligned} \quad (17)$$

where u , v and w denote displacements in the x , y and z directions, respectively. The displacements δ_1 , δ_2 and δ_3 are solutions obtained from a finite element analysis of the RVE subjected to a load at the boundary.

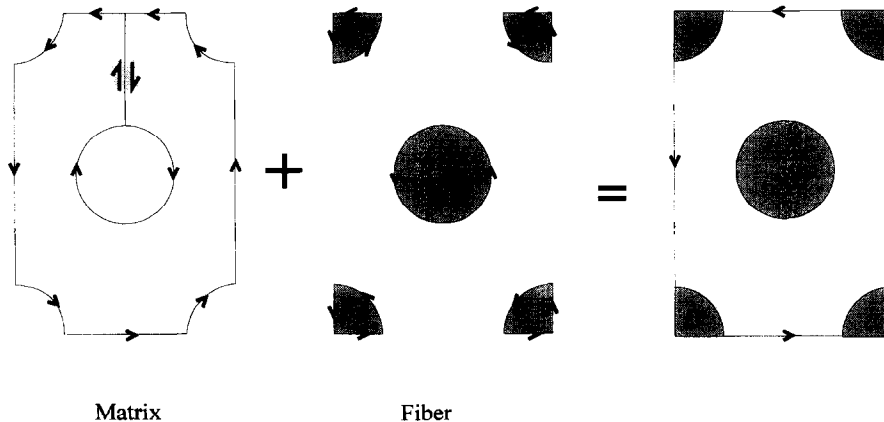


Fig. 3. Integration contour for hexagonal array.

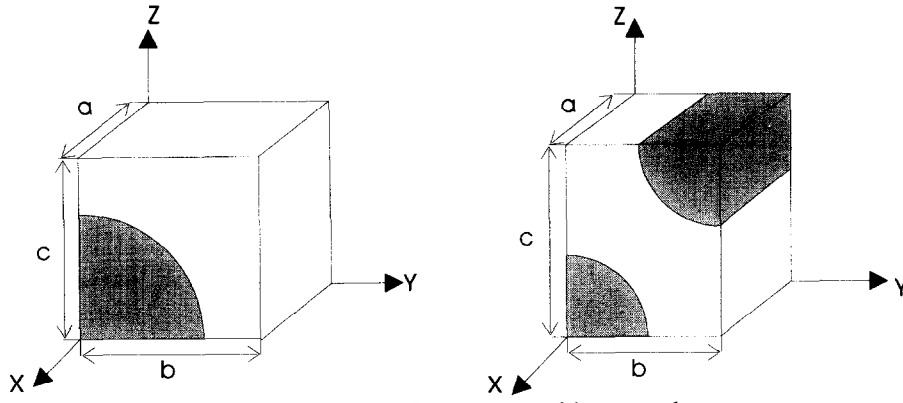


Fig. 4. RVE quadrants for square and hexagonal arrays.

For the case of an axial loading, P_1 , the average longitudinal strain calculated from eqn (14), reduces to the conventional definition of strain:

$$\bar{\epsilon}_{11} = \frac{1}{V} \int_S u_1 n_1 dS = \frac{\delta_1}{a} \quad (18)$$

The strain energy stored within the RVE is given by:

$$U = \frac{1}{2} \bar{\sigma}_{ij} \bar{\epsilon}_{ij} V$$

or

$$U = \frac{1}{2} \bar{\sigma}_{11} \bar{\epsilon}_{11} V \quad (19)$$

since $\bar{\sigma}_{11}$ is the only component of stress present.

External work done on the RVE by the applied load P_1 is given by:

$$W = \frac{1}{2} P_1 \delta_1 \quad (20)$$

Using the principle of strain energy equivalence between the stored energy and external work:

$$\frac{1}{2} P_1 \delta_1 = \frac{1}{2} \bar{\sigma}_{11} \bar{\epsilon}_{11} V \quad (21)$$

together with eqn (18), the average stress in the RVE is obtained as:

$$\bar{\sigma}_{11} = \frac{P_1}{bc} \quad (22)$$

Thus, in this case, the (volume) average stress $\bar{\sigma}_{11}$ is equal to the average traction on the surface $x = a$.

The longitudinal modulus and Poisson's ratio are given by:

$$E_1 = \frac{\bar{\sigma}_{11}}{\bar{\epsilon}_{11}} = \frac{P_1 a}{bc \delta_1} \quad \text{and} \quad \nu_{12} = -\frac{\bar{\epsilon}_{22}}{\bar{\epsilon}_{11}} = -\frac{\delta_2 a}{\delta_1 b} \quad (23)$$

Similarly, for a load P_1 acting transverse to the fiber direction at $y = b$:

$$E_2 = \frac{\bar{\sigma}_{22}}{\bar{\epsilon}_{22}} = \frac{P_1 b}{ac \delta_2} \quad \text{and} \quad \nu_{23} = -\frac{\bar{\epsilon}_{33}}{\bar{\epsilon}_{22}} = -\frac{\delta_3 b}{\delta_2 c} \quad (24)$$

4.2 Transverse shear loading

The stress and strain fields in a composite under a transverse shear loading are independent of the axial coordinate x (fiber direction) and are functions of y and z only. A two-dimensional generalized plain strain analysis can thus be used in the analysis of this type of loading. The RVE for the square array model is shown in Fig. 5. Naik⁷ and Brockenbrough *et al.*⁸ modeled transverse shear by assigning equal and opposite tractions to the faces normal to $y = b$ and $z = c$ and assuming the deformed RVE to remain a parallelogram with straight edges. This is an overly restrictive constraint. The deformed shape needs only to satisfy periodicity and symmetry conditions without necessarily remaining a parallelogram in the deformed configuration. The proper boundary conditions for the single RVE under transverse shear are determined by

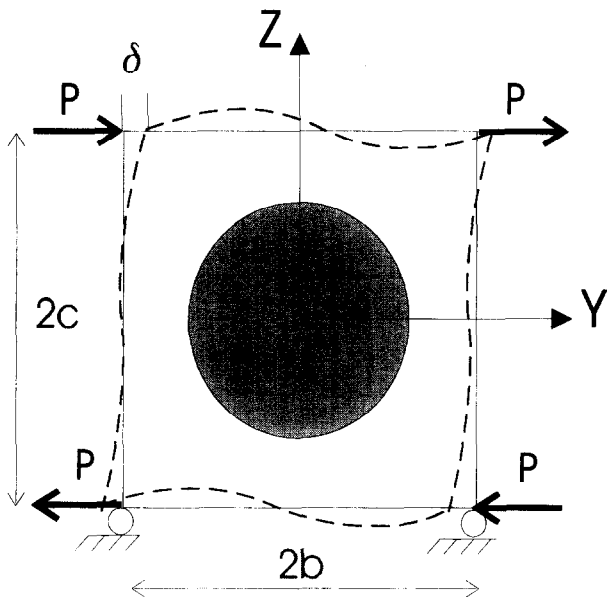


Fig. 5. RVE under transverse shear loading.

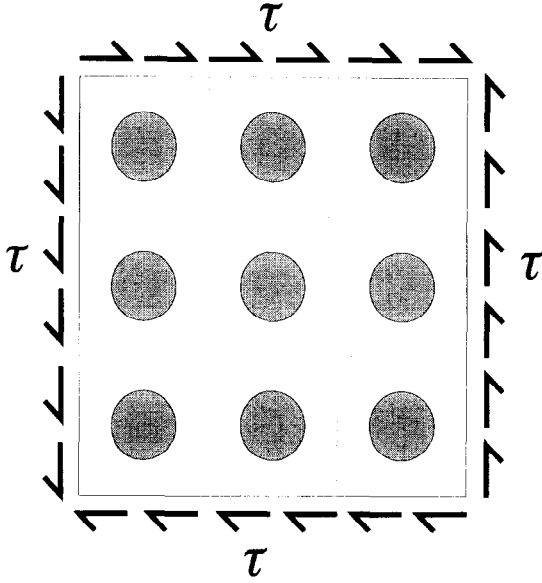


Fig. 6. Nine cell model under transverse shear loading.

first analysing a nine cell model subject to transverse shear load (Fig. 6). The center cell in this case is representative of a typical RVE in a composite as it is sufficiently removed from the boundary. The displacement field of this RVE is used to determine the boundary conditions to be applied to the single cell model.

The following boundary conditions are proposed for the RVE shown in Fig. 5:

$$\begin{aligned} v(-b, z) &= v(b, z) \\ w(-b, z) &= w(b, z) \\ v(y, -c) &= v(y, c) \\ w(y, -c) &= w(y, c) \end{aligned} \quad (25)$$

A further constraint is that the boundaries of the RVE undergo constant lateral displacement, i.e.

$$\epsilon_{zz}(\pm b, z) = 0 \quad \text{or} \quad w(\pm b, z) = \delta_1 \quad (26)$$

$$\epsilon_{yy}(y, \pm c) = 0 \quad \text{or} \quad v(y, \pm c) = \delta_2 \quad (27)$$

To simulate transverse shear loading, a load P is applied to each corner of the RVE (Fig. 5). The bottom corners are placed on rollers to eliminate rigid body displacement ($\delta_1 = 0$). A unit length is assumed in the fiber direction in order to satisfy dimensional requirements. Using eqns (14) and (25)–(27), average transverse shear strain is obtained as:

$$\bar{\gamma}_{23} = \frac{1}{V} \int_V \gamma_{23} dV = \frac{1}{4bc} \times 4\delta_2 b = \frac{\delta_2}{c} \quad (28)$$

Equating external work to strain energy in the system, we get:

$$4 \times \frac{1}{2} P \delta_2 = \frac{1}{2} \bar{\sigma}_{23} \bar{\gamma}_{23} V \quad (29)$$

Using eqns (28) and (29), average transverse shear stress and shear modulus are obtained as:

$$\bar{\sigma}_{23} = \frac{P}{b} \quad (30)$$

$$G_{23} = \frac{\bar{\sigma}_{23}}{\bar{\gamma}_{23}} = \frac{Pc}{b\delta_2} \quad (31)$$

4.3 Longitudinal shear loading

Zhang and Evans¹⁰ modeled longitudinal shear loading for a composite cylinder RVE assuming a constant shear loading of the type:

$$\epsilon_{rz}^c = \epsilon_{\theta z}^c = \frac{1}{2} \gamma_L \quad (32)$$

Such a loading condition implicitly assumes that $\gamma_L^{\text{fiber}} = \gamma_L^{\text{matrix}}$. This is incorrect, since the fiber, being much stiffer than the matrix, should exhibit less shear strain.

The strain field in a composite subjected to longitudinal loading is two-dimensional in nature, i.e. it is independent of the axial coordinate (x coordinate). To impose this constraint in the RVE, the top and bottom faces of the RVE are required to undergo identical displacement, i.e. points on the top ($x = a$) and bottom ($x = 0$) faces with the same y and z coordinates are constrained to have the same displacements in all three directions. Thus, for the RVE shown in Fig. 7:

$$\begin{aligned} u(0, y, z) &= u(a, y, z) \\ v(0, y, z) &= v(a, y, z) \\ w(0, y, z) &= w(a, y, z) \end{aligned} \quad (33)$$

From symmetry conditions, the additional constraints on the RVE are:

$$\begin{aligned} u(x, 0, z) &= 0 \\ v(x, 0, z) &= 0 \\ w(x, 0, z) &= 0 \\ u(x, 2b, z) &= \delta \\ v(x, 2b, z) &= 0 \end{aligned} \quad (34)$$

Similar to the case of transverse shear loading, a nine cell model of the composite is analysed to verify the boundary conditions on the center cell.

Following Gauss theorem, average longitudinal shear strain is given by:

$$\begin{aligned} \bar{\gamma}_{12} &= \frac{1}{V} \int_V \gamma_{12} dV = \frac{2}{V} \int_V \epsilon_{12} dV \\ &= \frac{1}{V} \int_S (u_1 n_2 + u_2 n_1) dS \end{aligned} \quad (35)$$

For the boundary conditions in eqns (34) and (35) this reduces to:

$$\bar{\gamma}_{12} = \frac{\delta}{2b} \quad (36)$$

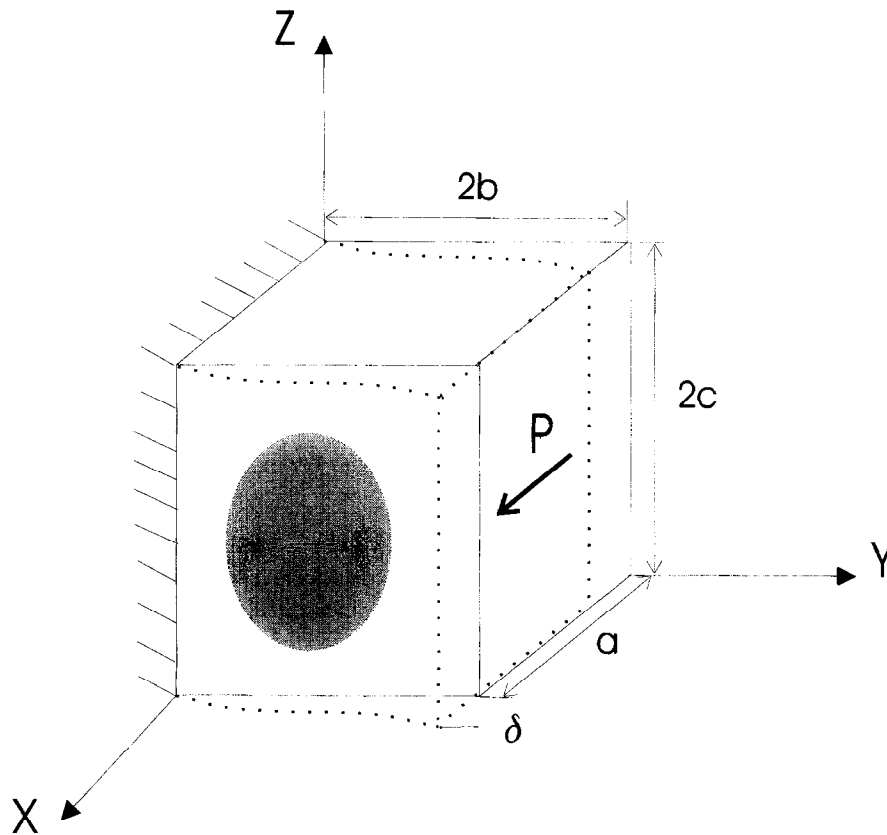


Fig. 7. RVE under longitudinal shear loading.

Equating external work done to strain energy in the system:

$$\frac{1}{2} P \delta = \frac{1}{2} \bar{\sigma}_{12} \bar{\gamma}_{12} V \quad (37)$$

Using eqns (36) and (37), average stress and longitudinal shear modulus are given by:

$$\bar{\sigma}_{12} = \frac{P}{2ac} \quad (38)$$

$$G_{12} = \frac{\bar{\sigma}_{12}}{\bar{\gamma}_{12}} = \frac{Pb}{ac\delta} \quad (39)$$

5 COMPARISON OF ELASTIC CONSTANTS

The finite element predictions of the elastic moduli are compared with analytical solutions and available experimental data. It is noted that the analytical result of Hashin and Rosen,¹ based on energy variational principles, provides bounds for the elastic moduli. For E_1 , G_{12} and ν_{12} these bounds coincide to provide an exact solution. The solution presented by Whitney and Riley² is based on the use of the energy balance approach with the aid of classical elasticity theory. Sun and Chen¹⁷ and Chamis¹² presented solutions based on a mechanics approach involving the use of displacement continuity and force equilibrium conditions. Results for boron/aluminum and AS4/3501-6

Table 1. Elastic moduli for boron/aluminum composite (fiber volume fraction = 0.47)

Elastic constants (GPa)	FEM square array	FEM hexagonal array	Ref. 17	Ref. 12	Ref. 2	Ref. 1 ^a	Experiment ¹³
E_1	215	215	214	214	215	215	216
E_2	144	136.5	135	156	123	139.1 (131.4)	140
G_{12}	57.2	54.0	51.1	62.6	53.9	53.9	52
G_{23}	45.9	52.5	—	43.6	—	54.6 (50.0)	—
ν_{12}	0.19	0.19	0.19	0.20	0.19	0.195	0.29
ν_{23}	0.29	0.34	—	0.31	—	0.31 (0.28)	—

^a Numbers in parentheses indicate lower bounds.

Table 2. Elastic moduli for AS4/3501-6 composite (fiber volume fraction = 0.6)

Elastic constants (GPa)	FEM square array	FEM hexagonal array	Ref. 17	Ref. 12	Ref. 2	Ref. 1 ^a	Experiment ¹⁵	Experiment ¹⁶
E_1	142.6	142.6	142.9	142.9	142.9	142.9	142	139
E_2	9.60	9.20	9.20	9.79	9.78	9.40 (9.10)	10.30	9.85
G_{12}	6.00	5.88	5.50	6.53	5.80	5.80	7.60	5.25
G_{23}	3.10	3.35	—	3.01	—	3.42 (3.26)	3.8	—
ν_{12}	0.25	0.25	0.26	0.26	0.25	0.25	—	0.3
ν_{23}	0.35	0.38	—	0.42	—	0.39 (0.37)	—	—

^a Numbers in parentheses indicate lower bounds.

Table 3. Material properties for boron and aluminum

Ref. 13	E (GPa)	ν
Boron	379.3	0.1
Aluminum	68.3	0.3

graphite/epoxy composites are given in Tables 1 and 2, respectively. The corresponding constituent properties are presented in Tables 3 and 4, respectively.

In general, good agreement is observed between the finite element predictions and experimental data for both material systems. In the case of graphite/epoxy, a greater deviation is observed in the longitudinal shear modulus. This could be due to the fact that the properties of the transversely isotropic graphite fiber reported in the literature exhibit a wide range of scatter, especially for the moduli E_2 and G_{12} .

6 CONCLUSION

The appropriate constraints on the RVE under various loadings have been determined from symmetry and periodicity conditions. Average strain and stress for the RVE are defined by using the Gauss theorem and energy equivalence principles, and the complete set of elastic constants for a unidirectional composite have been obtained. The elastic moduli obtained from the analysis for both square and hexagonal arrays seem adequate in predicting elastic moduli of the composite.

Table 4. Material properties of fiber and matrix

Ref. 14	E_1 (GPa)	E_2 (GPa)	G_{12} (GPa)	ν_{12}	ν_{23}
AS4	235	14	28	0.2	0.25
3501-6	4.8	4.8	1.8	0.34	0.34

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