IMPLICATIONS OF BOUNDARY CONDITIONS OF UNIT CELLS FOR MICROMECHANICAL ANALYSIS

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Abstract

The most important aspect of formulating unit cells for micromechanical analysis of materials of patterned microstructures is the derivation of appropriate boundary conditions. There is lack of a comprehensive account on the derivation of boundary conditions in the literature. This paper is devoted to the generation of such an account, where boundary conditions are derived entirely based on considerations of symmetries which are present in the microstructure. The implications of the boundary conditions used for a unit cell are not always clear and therefore have been discussed. It has been demonstrated that unit cells of the same appearance but subject to boundary conditions derived based on different symmetry considerations may behave rather differently. One of the objectives of the paper is to inform users of unit cells that to introduce a unit cell one needs not only mechanically correct boundary conditions but also a clear sense of the microstructure under consideration.

1 Introduction

Micromechanical analyses have been on an increasing trend in order to understand the behaviour of modern materials with sophisticated micro-structures. Unit cells are often resorted to in order to facilitate such analyses. The introduction of a unit cell is usually based on certain assumptions, such as a regular pattern in the microstructure, which is sometimes a reasonable approximation, or an idealisation otherwise. A regular pattern offers certain symmetries which can then be employed to define the unit cell and to derive the boundary conditions for it for micromechanical analysis. Several accounts of the systematic use of symmetries for the derivation of the boundary conditions for unit cells have been presented by the author in [1-3]. In the literature, there are many accounts where simplistic boundary conditions have been imposed to unit cells in an intuitive manner, sometimes, rather casually without much justification. In [4], boundary conditions have been so introduced that boundary effects have been considered and a significant effort has been made to include additional cells to form larger unit cells in order to reduce the boundary effects. This would be absolutely unnecessary, had the boundary conditions been derived appropriately. In many publications [4-9], to name but a few, boundary conditions have been so assumed that boundaries have to remain flat or straight after deformation in order to deliver simple boundary conditions, which cannot usually be fulfilled when the material is subjected to the macroscopic shear deformation. Such simplistic boundary conditions are correct in a few special cases, e.g. square unit cells with reflectional symmetric microstructure when they are subjected to a deformation corresponding to a macroscopic direct strain. Even so, there are implications on the permissible patterns of the microstructures, which do not seem to have been given any attention hitherto. Another confusing issue is how many boundary conditions need to be prescribed at any given part of the boundary of a unit cell. Sometimes, only one displacement has been prescribed but in other cases more than one are prescribed. In [10], equilibrium or compatibility conditions were imposed as a part of boundary conditions, which are in fact wrong, as will be explained later in the next section. This paper is devoted to the issues as raised above, in particular, to the confusing issues associated with the use of reflectional symmetries.

Because of the nature of the symmetries employed, the boundary conditions obtained for the unit cells are often in a form of equations relating displacements on one part of the boundary to those on another, referred to hereafter as *equation* *boundary conditions*, because of the use of translational or rotational symmetries [1-3]. This may impose restrictions on the applications of these boundary conditions and hence the unit cells. For instance, when finite elements are employed for the micromechanical analysis, as is often the case, the mesh to be generated must possess identical tessellation between the parts of boundary which are related through those equation boundary conditions. This could sometimes be difficult to achieve for 3-D problems, such as in particle reinforced or textile composites. The constraints in equation form may not be available in some FE codes. It is therefore desirable to avoid such equation boundary conditions whenever possible.

2 The Concept of Natural Boundary Conditions

Some of the confusions in deriving boundary conditions for unit cells result from the use of finite elements which is usually based on a variational principle of some kind in which some boundary conditions, called *natural boundary conditions*, are satisfied automatically as a part of the variation process. The natural boundary condition is a mathematical terminology commonly used in variational principles [11]. The spirit of a variational principle is that the conditions for a functional to take its stationary value are equivalent to the satisfaction of the Euler equations and the natural boundary conditions corresponding to the functional. In the context of the minimum total potential energy principle, the Euler equations are equilibrium equations of elasticity and the natural boundary conditions are the traction boundary conditions. Almost all commercial FE codes are based on the minimum total potential energy principle or its counterpart, the virtual displacement principle, in which traction boundary conditions will be satisfied in the same way and at the same time as the equilibrium equations are satisfied when the total potential energy is minimised.

It should be emphasised that natural boundary conditions should not be imposed prior to the variation process, especially when seeking an approximate solution, e.g. using finite elements. It does not help to obtain a more accurate result but, rather on the contrary, it may prevent the total potential energy reaching its minimum in the solution space and hence lead to a wrong result. The confusion associated with natural boundary conditions arises, perhaps, from the way they are described in textbooks. They are often said to be the kind of boundary conditions which do not have to be satisfied when using a variational principle. This can therefore be understood by some users in such a way that if these boundary conditions had been satisfied *a priori*, one might expect a better approximation. This is wrong. A more precise description of natural boundary conditions should state that they should not be imposed, as they will be satisfied automatically by the variational principle. The imposition of natural boundary conditions prior to application of the variational principle will result in no better approximation, in general. Rigorously speaking, imposition of natural boundary conditions prior to variation is not a matter of the level of approximation. Rather, it violates the integrity of the minimum total potential energy principle and is hence wrong.

3 Sufficient and Necessary Number of Boundary Conditions for Unit Cells

In the literature, it is often found, e.g. in [12], that the number of boundary conditions prescribed at the same part of the boundary varies from case to case. Without appropriate justification, it is rather confusing. As a result, incorrect usages are often found, e.g. in [4,10]. According to the theory of continuum mechanics for the deformation problem of materials in 3-D space, at any given point on the boundary, three prescribed boundary conditions are required in any logical combination of displacements and tractions. For instance, for a boundary perpendicular to the x-axis, the three boundary conditions can be a prescription of the following

$$\left\{\begin{array}{lll} u & \text{or} & \sigma_x \quad \text{in the } x\text{-direction} \\ v & \text{or} & \tau_{xy} \quad \text{in the } y\text{-direction} \\ w & \text{or} & \tau_{xz} \quad \text{in the } z\text{-direction} \end{array}\right. \tag{1}$$

where u, v and w are displacements in x, y and z directions respectively and σ and τ are direct and shear stress components with subscripts in their conventional sense.

When the boundary conditions are imposed in the form of equations relating the displacements or tractions on one part of the boundary to those of another part of the boundary, the equation boundary conditions should be imposed to the following

$$\left\{\begin{array}{lll} u & \text{and} & \sigma_x \\ v & \text{and} & \tau_{xy} \\ w & \text{and} & \tau_{xz}\,. \end{array}\right. \tag{2}$$

Instead of three boundary conditions on one part of the boundary, there are six boundary conditions for two parts of the boundary.

Bearing in mind that traction boundary conditions are natural boundary conditions in conventional FE analyses, they will be left out of the prescription list. For example, if part of the boundary is subjected to prescribed u, τ_{xy} & τ_{xz} it is sufficient and necessary to prescribe u only on this part of boundary for the FE analysis. Any non-zero traction should be included as externally applied load rather than boundary conditions in an FE analysis.

Applying the same argument to equation boundary conditions, it is obvious that equation constraints have to be imposed to all three displacements to be both sufficient and necessary, whereas equations for tractions can and should be left out, as in [2,3].

Because of the existence of natural boundary conditions which should not be imposed, the same part of the boundary under different loading cases may be subjected to different numbers of boundary conditions. This causes confusions, often in connection to difference in the nature of symmetry. The loading and deformation can be symmetric as well as anti-symmetric. Distinguishing one from another is essential when deriving appropriate boundary conditions associated with symmetry. For example, when a deformable body symmetric about the x-plane (x=0) is subjected to symmetric loading, e.g. stretching in the x-direction, there is only one boundary condition on the symmetry plane, i.e. $u=0$ while the two remaining traction boundary conditions, $\tau_{xy}=\tau_{xz}=0$, should not be prescribed. However, when the same body is subjected to anti-symmetric loading, e.g. shear in the x-y plane, there will be two boundary conditions on the symmetry plane, i.e. $v=0$ and $w=0$ and there is only one traction boundary condition, $\sigma_x=0$, in this case, which should not be imposed.

To conclude this section, it is clear that at a boundary of a unit cell, the number of boundary conditions to be imposed before a finite element analysis can be conducted is not definite. It depends on the nature of the symmetries adopted in the definition of the unit cell. However, one thing remains definite when introducing boundary conditions. It is that only displacement boundary conditions should be imposed, not the natural boundary conditions. When bending is involved, for instance in classical laminate theory, displacements should include all generalised displacements, i.e. translational displacements and rotational displacements. The natural boundary conditions in this case are associated with membrane forces, bending moments and transverse shear forces.

4 Selection of Unit Cells and Their Implications

For argument's sake, a microstructure in 2-D space of a square layout as shown in Fig. 1a is considered first, which can be perceived as, but not restricted to, a transverse cross-section of a UD composite or an in-plane pattern of a textile composite. As the only symmetries available are translations, in the x and y directions, respectively, the unit cell as shown in Fig. 1b will have to be subjected to equation boundary conditions as given in [2] relating displacements on opposite sides of the unit cell while ignoring the traction conditions.

However, if the material under consideration allows one to idealise it into a microstructure as shown in Fig. 2a, the repetitive cell as shown in Fig. 2b would be the unit cell of smallest size if only translational symmetries are employed. Obviously, the size of the unit cell can be reduced to that as shown in Fig. 2c after the available reflectional symmetries about x and y axes have been utilised. As a result, boundary conditions can be obtained without equations relating the displacements on the opposite sides of the cell. Having used the reflectional symmetries, one needs to bear in mind two issues associated with a unit cell, as shown in Fig. 2c, which can be easily overlooked. Firstly, the microstructure of the material the unit cell in Fig. 2c is given in Fig. 2a not as shown in Fig. 1a although the appearance of the unit cells in Fig. 1b and Fig. 2c look identical. Secondly, some macroscopic strain states, in particular, associated with shear, are anti-symmetric under the reflectional symmetry transformations. Appropriate considerations should be given to the anti-symmetric nature when boundary conditions are derived from the symmetry transformations. As a result, the number of boundary conditions for some loading cases would be different from those for the other cases.

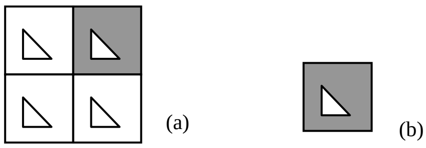


Fig. 1 Square packing

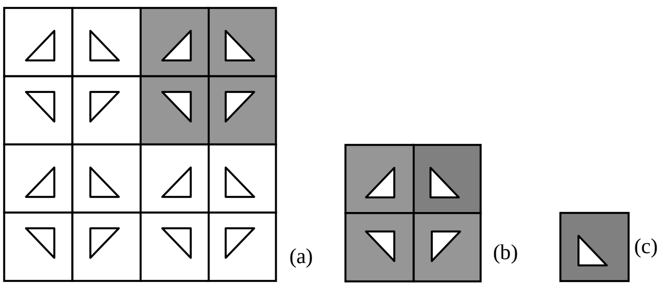


Fig. 2 Square packing with further reflectional symmetries

The ultimate unit cells obtained from Fig.1 and Fig.2 share the same appearance. However, they are subject to different boundary conditions and are associated with different microstructures. An obvious consequence of the difference in the microstructure is that the one in Fig.2a is macroscopically orthotropic while that in Fig. 1a is not necessarily the case, as will be seen later through an example. Users of unit cells should be aware of the difference and decide if the difference has any significance for their particular applications while choosing the unit cell to be employed.

Another regular pattern often encountered in the literature is hexagonal. Arguments, similar to those above for the square pattern, apply to a large extent. The only difference is that there are more ways to express the translational symmetries as discussed fully in [1,2]. Whether the repetitive cell, e.g. the rectangle or any of the hexagons shown in Fig.3, used to express the translation symmetries, can be further reduced in size depends on the existence of other symmetries, reflectional and rotational. Without such additional symmetries, the smallest size would be a complete hexagon as shown in Fig.3, if one is prepared to employ translations in directions that are not perpendicular to each other. Otherwise, to involve orthogonal translations in *x* and *y* directions only, one will have to deal with a unit cell having a bigger size, as shown in the rectangle in Fig.3, which is obviously not unique. When analysing these unit cells, in general, equation boundary conditions will have to be employed.

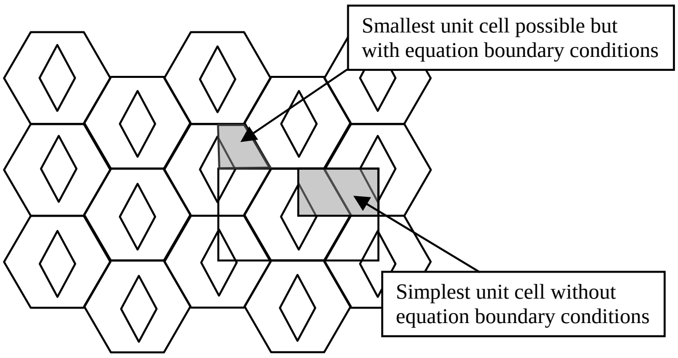


Fig. 3 Hexagonal packing with reflectional symmetries

5 Boundary conditions for a unit cell from 3-D microstructure with reflectional symmetries

Consider the case illustrated in Fig. 2 in a 3-D scenario. The boundary conditions can be derived in general as follows, assuming the periods of translational symmetries in the *x*, *y* and *z* directions are $2b_x$, $2b_y$ and $2b_z$, respectively. This is general enough to encapsulate regular packing layouts such as simple cubic, body centred cubic, face centred cubic and close packed hexagonal [3].

Assume there exists an intermediate repetitive cell equivalent to that in Fig. 2b which can represent the material fully using translational symmetries only and this cell is defined in the domain

$$-b_x \le x \le b_x \qquad -b_y \le x \le b_y \qquad -b_z \le x \le b_z. \tag{3}$$

The material is subjected to a set of macroscopic strains $\left\{\varepsilon_x^0, \varepsilon_y^0, \varepsilon_z^0, \gamma_{yz}^0, \gamma_{zx}^0, \gamma_{xy}^0\right\}$ which can be introduced as six extra degrees of freedom (d.o.f.) in an FE analysis, e.g. as six individual nodes, each having a single d.o.f., or six degrees of freedom of a special node. Each of them can be prescribed to achieve a macroscopically uniaxial strain state. Alternatively, upon any of these extra d.o.f.'s, a concentrated force can be applied in order to impose a macroscopic stress while leaving the others free in order to produce a macroscopically uniaxial stress state. The latter is certainly more desirable in most cases as a macroscopically uniaxial stress state is what one would need in order to measure an effective property of the composite.

The translational symmetries require:

$$\begin{aligned} u|_{x=b_x} - u|_{x=-b_x} &= 2b_x\varepsilon_x^0 \\ v|_{x=b_x} - v|_{x=-b_x} &= 0 \\ w|_{x=b_x} - w|_{x=-b_x} &= 0 \end{aligned} \quad \text{and} \quad \begin{aligned} \sigma_x|_{x=b_x} - \sigma_x|_{x=-b_x} &= 0 \\ \tau_{xy}|_{x=b_x} - \tau_{xy}|_{x=-b_x} &= 0 \\ \tau_{xz}|_{x=b_x} - \tau_{xz}|_{x=-b_x} &= 0 \end{aligned}$$

under translation in *x*-direction; (4)

$$\begin{aligned} u|_{y=b_y} - u|_{y=-b_y} &= 2b_y\gamma_{xy}^0 \\ v|_{y=b_y} - v|_{y=-b_y} &= 2b_y\varepsilon_y^0 \\ w|_{y=b_y} - w|_{y=-b_y} &= 0 \end{aligned} \quad \text{and} \quad \begin{aligned} \tau_{yx}|_{y=b_y} - \tau_{yx}|_{y=-b_y} &= 0 \\ \sigma_y|_{y=b_y} - \sigma_y|_{y=-b_y} &= 0 \\ \tau_{yz}|_{y=b_y} - \tau_{yz}|_{y=-b_y} &= 0 \end{aligned}$$

under translation in *y*-direction, (5)

$$\begin{aligned} u|_{z=b_z} - u|_{z=-b_z} &= 2b_z\gamma_{xz}^0 \\ v|_{z=b_z} - v|_{z=-b_z} &= 2b_z\gamma_{yz}^0 \\ w|_{z=b_z} - w|_{z=-b_z} &= 2b_z\varepsilon_z^0 \end{aligned} \quad \text{and} \quad \begin{aligned} \tau_{zx}|_{z=b_z} - \tau_{zx}|_{z=-b_z} &= 0 \\ \tau_{zy}|_{z=b_z} - \tau_{zy}|_{z=-b_z} &= 0 \\ \sigma_z|_{z=b_z} - \sigma_z|_{z=-b_z} &= 0 \end{aligned}$$

under translation in *z*-direction. (6)

The form of many of the above equations is not unique, especially, those associated with shear, depending on the way rigid body rotations are constrained. The lack of uniqueness here also contributes to the likelihood of confusion when introducing boundary conditions for unit cells.

To apply further reflectional symmetries about *x*, *y* and *z* planes, the problem has to be considered separately for individual loading cases expressed in terms of $\left\{\sigma_x^0, \sigma_y^0, \sigma_z^0, \tau_{yz}^0, \tau_{zx}^0, \tau_{xy}^0\right\}$, as presented in the following subsections.

5.1 Under σ_x^0

Consider first the x-faces of the unit cell, i.e. those perpendicular to the x-axis. σ_x^0 as a stimulus is symmetric under reflection about x-plane (perpendicular to x-axis). Responses v, w and σ_x are symmetric while u, τ_{xy} and τ_{xz} are anti-symmetric. On the symmetry plane (x=0), the symmetry conditions require

$$\begin{aligned} u|_{x=0} &= -u|_{x=0} \\ v|_{x=0} &= v|_{x=0} \\ w|_{x=0} &= w|_{x=0} \end{aligned} \quad \text{and} \quad \begin{aligned} \sigma_x|_{x=0} &= \sigma_x|_{x=0} \\ \tau_{xy}|_{x=0} &= -\tau_{xy}|_{x=0} \\ \tau_{xz}|_{x=0} &= -\tau_{xz}|_{x=0} \end{aligned} \tag{7}$$

In the above, the conditions on $v|_{x=0}$, $w|_{x=0}$ and $\sigma_x|_{x=0}$ do not yield any constraints and they should hence be left free. In (7), there are three boundary conditions in effect. However, only the displacement boundary condition should be imposed on side $x=0$, i.e.

$$u|_{x=0} = 0 \tag{8}$$

while $\tau_{xy}|_{x=0} = \tau_{xz}|_{x=0} = 0$ are natural boundary conditions and should not be imposed. The same argument will be adopted hereafter without referring to their nature of being natural boundary conditions.

Considering the opposite faces at $x = \pm b_x$, and applying the symmetry condition, one has

$$\begin{aligned} u|_{x=b_x} &= -u|_{x=-b_x} \\ v|_{x=b_x} &= v|_{x=-b_x} \\ w|_{x=b_x} &= w|_{x=-b_x} \end{aligned} \quad \text{and} \quad \begin{aligned} \sigma_x|_{x=b_x} &= \sigma_x|_{x=-b_x} \\ \tau_{xy}|_{x=b_x} &= -\tau_{xy}|_{x=-b_x} \\ \tau_{xz}|_{x=b_x} &= -\tau_{xz}|_{x=-b_x} \end{aligned} \quad . \tag{9}$$

In conjunction with the translational symmetry conditions as given in (4), one obtains the only remaining boundary condition on side $x = b_x$

$$u|_{x=b_x} = b_x \varepsilon_x^0 \ . \tag{10}$$

The boundary condition above introduces an extra d.o.f. ε_x^0 into the system. In an FE analysis, it can be prescribed in order to prescribe a macroscopically uniaxial strain state ε_x^0. However, if one wishes to impose a macroscopically uniaxial stress state σ_x^0, an appropriate concentrated force can be applied to this d.o.f.. The macroscopically effective stress σ_x^0 can be worked out from the concentrated force easily as discussed in [3], while the nodal displacement at this extra d.o.f. gives the effective macroscopic strain ε_x^0 directly.

Consider now the y-faces. The stimulus σ_x^0 is also symmetric under reflection about y-plane (perpendicular to y-axis). Responses u, w and σ_y are symmetric while v, τ_{yx} and τ_{yz} are anti-symmetric about y-plane. Hence, on the symmetry plane (y=0) the symmetry conditions require

$$\begin{aligned} u|_{y=0} &= u|_{y=0} \\ v|_{y=0} &= -v|_{y=0} \\ w|_{y=0} &= w|_{y=0} \end{aligned} \quad \text{and} \quad \begin{aligned} \tau_{yx}|_{y=0} &= -\tau_{yx}|_{y=0} \\ \sigma_y|_{y=0} &= \sigma_y|_{y=0} \\ \tau_{yz}|_{y=0} &= -\tau_{yz}|_{y=0} \end{aligned} \tag{11}$$

A single boundary condition on side $y=0$ is obtained

$$v|_{y=0} = 0 \ . \tag{12}$$

The symmetry conditions on the two opposite faces at $y = \pm b_y$ require

$$\begin{aligned} u|_{y=b_y} &= u|_{y=-b_y} \\ v|_{y=b_y} &= -v|_{y=-b_y} \\ w|_{y=b_y} &= w|_{y=-b_y} \end{aligned} \quad \text{and} \quad \begin{aligned} \tau_{yx}|_{y=b_y} &= -\tau_{yx}|_{y=-b_y} \\ \sigma_y|_{y=b_y} &= \sigma_y|_{y=-b_y} \\ \tau_{yz}|_{y=b_y} &= -\tau_{yz}|_{y=-b_y} \end{aligned} \quad . \tag{13}$$

A single boundary condition for side $y = b_y$

$$v|_{y=b_y} = b_y \varepsilon_y^0 \ . \tag{14}$$

The boundary condition above introduces another extra d.o.f. ε_y^0 into the system. To impose a uniaxial macroscopic stress σ_x^0, the d.o.f. ε_y^0 should be left free, so that $\sigma_y^0 = 0$. The nodal displacement at the extra d.o.f. ε_y^0 gives this macroscopic strain directly produced by σ_x^0 as a result of Poisson effect, from which the effective Poisson ratio can be easily evaluated. On the other hand, this extra d.o.f. can be prescribed to impose a macroscopic strain ε_y^0, or a concentrated force can be applied to it to impose a macroscopic stress σ_y^0.

Applying the same arguments to the z-faces, the boundary conditions on sides $z=0$ and $z=b_z$ can be obtained as

$$w|_{z=0} = 0 \quad \text{and} \quad w|_{z=b_z} = b_z \varepsilon_z^0 \ , \text{ respectively,} \tag{15}$$

where the extra d.o.f. ε_z^0 was introduced through translational symmetry conditions (6). To impose a macroscopic stress σ_x^0 alone, ε_z^0 should be left free, so that $\sigma_z^0 = 0$. The nodal displacement at the extra d.o.f. ε_z^0 gives this macroscopic strain directly. Alternatively, it can be prescribed accordingly in order to impose a macroscopic stress or strain in this direction.

To summarise, under a macroscopic stress σ_x^0, the boundary conditions on the three pairs of the sides of the unit cell are given by (8), (10), (12), (14) and (15), namely

$$
\begin{aligned}
u|_{x=0} &= 0 \quad \text{and} \quad u|_{x=b_x} = b_x\varepsilon_x^0 \\
v|_{y=0} &= 0 \quad \text{and} \quad v|_{y=b_y} = b_y\varepsilon_y^0 \\
w|_{z=0} &= 0 \quad \text{and} \quad w|_{z=b_z} = b_z\varepsilon_z^0
\end{aligned}
\tag{16}
$$

where the extra d.o.f. ε_x^0 is subjected to a concentrated force associated with σ_x^0, while ε_y^0 and ε_z^0 should be left free to produce a macroscopically uniaxial stress state σ_x^0.

5.2 Under σ_y^0

With similar considerations as given above, the boundary conditions for the unit cell under σ_y^0 are identical to those in (16). The only difference is that it should be the extra d.o.f. ε_y^0 that is subjected to a concentrated force associated with σ_y^0, while ε_x^0 and ε_z^0 are left free to produce a macroscopically uniaxial stress state σ_y^0. The nodal displacements at those extra d.o.f.'s give the corresponding macroscopic strains directly.

5.3 Under σ_z^0

The boundary conditions are again identical to those in (16). However, the extra d.o.f. ε_z^0 should be subjected to a concentrated force associated with σ_z^0, while ε_x^0 and ε_y^0 are left free to produce a macroscopically uniaxial stress state σ_z^0.

5.4 Under τ_{yz}^0

The nature of shear stresses is slightly more complicated than their direct counterparts. With respect to a reflectional symmetry, one of the three shear components is symmetric while other two are anti-symmetric. Under the reflection about the *x*-plane, the stimulus τ_{yz}^0 is symmetric. The responses *v*, *w* and σ_x are symmetric while *u*, τ_{xy} and τ_{xz} are anti-symmetric. Hence, on the symmetry plane, *x*=0, the symmetry conditions require

$$
\begin{aligned}
u|_{x=0} &= -u|_{x=0} \qquad & \sigma_x|_{x=0} &= \sigma_x|_{x=0} \\
v|_{x=0} &= v|_{x=0} \qquad \text{and} & \tau_{xy}|_{x=0} &= -\tau_{xy}|_{x=0} \\
w|_{x=0} &= w|_{x=0} \qquad & \tau_{xz}|_{x=0} &= -\tau_{xz}|_{x=0}
\end{aligned}
\tag{17}
$$

The only boundary condition to be imposed is

$$u|_{x=0} = 0 . \tag{18}$$

On the opposite faces at $x = \pm b_x$, the reflectional symmetry conditions are similar to (17) but on $x = \pm b_x$ instead of *x*=0. In conjunction with the translational symmetry conditions (4), they lead to the boundary condition

$$u|_{x=b_x} = 0 . \tag{19}$$

Consider now the pair of sides parallel to the *y*-plane. The stimulus τ_{yz}^0 is anti-symmetric about *y*-plane (*y*=0). The responses *u*, *w* and σ_y are symmetric while *v*, τ_{yx} and τ_{yz} are anti-symmetric. Hence, on the symmetry plane, the symmetry conditions require

$$
\begin{aligned}
u|_{y=0} &= -u|_{y=0} \qquad & \tau_{yx}|_{y=0} &= \tau_{yx}|_{y=0} \\
v|_{y=0} &= v|_{y=0} \qquad \text{and} & \sigma_y|_{y=0} &= -\sigma_y|_{y=0} \\
w|_{y=0} &= -w|_{y=0} \qquad & \tau_{yz}|_{y=0} &= \tau_{yz}|_{y=0} .
\end{aligned}
\tag{20}
$$

The boundary conditions on *y*=0 are obtained as

$$u|_{y=0} = w|_{y=0} = 0 . \tag{21}$$

Notice that there are two displacement boundary conditions in this case as opposed to the *x*=0 plane on which there is only one boundary condition as given in (19). They have to be imposed in order to define the unit cell properly under this loading condition. There is one traction boundary condition $\sigma_y|_{y=0} = 0$ which has been ignored as a natural boundary condition.

Applying the reflectional symmetry to the two opposite faces at $y = \pm b_y$, one obtains

$$
\begin{aligned}
u|_{y=b_y} &= -u|_{y=-b_y} \qquad & \tau_{yx}|_{y=b_y} &= \tau_{yx}|_{y=-b_y} \\
v|_{y=b_y} &= v|_{y=-b_y} \qquad \text{and} & \sigma_y|_{y=b_y} &= -\sigma_y|_{y=-b_y} \\
w|_{y=b_y} &= -w|_{y=-b_y} \qquad & \tau_{yz}|_{y=b_y} &= \tau_{yz}|_{y=-b_y} .
\end{aligned}
\tag{22}
$$

which lead to the following boundary conditions for side $y = b_y$

$$u|_{y=b_y} = w|_{y=b_y} = 0 . \tag{23}$$

Similarly, the boundary conditions on *z*=0 and $z = b_z$ can be obtained, bearing in mind that

τ_{yz}^0 is anti-symmetric about *z*-plane

$$u|_{z=0} = v|_{z=0} = 0$$

$$u|_{z=b_z} = 0 \quad \text{and} \quad v|_{z=b_z} = b_z \gamma_{yz}^0 \tag{24}$$

where the extra d.o.f. γ_{yz}^0 is introduced through the translational symmetry conditions (6), which can be associated with $u|_{z=b_z}$ instead of $v|_{z=b_z}$ if the rigid body rotation of the unit cell is constrained differently. There will be no difference whatsoever as far as the deformation is concerned, provided that it has been dealt with correctly. The same applies to the consideration of the two subsequent loading cases without further explanation. To impose a macroscopic stress τ_{yz}^0, a concentrated force can be applied to the d.o.f. γ_{yz}^0. The nodal displacement at γ_{yz}^0, obtained after the analysis, gives the corresponding macroscopic strain directly. Since *w* is not constrained on $z=0$ and $z=b_z$, these faces do not have to remain flat after deformation.

As a summary, all boundary conditions for the unit cell under macroscopic stress τ_{yz}^0 are as follows

$$u|_{x=0} = 0, \quad u|_{x=b_x} = 0$$

$$u|_{y=0} = w|_{y=0} = 0, \; u|_{y=b_y} = w|_{y=b_y} = 0 \tag{25}$$

$$u|_{z=0} = v|_{z=0} = 0, \; u|_{z=b_z} = 0 \;\; \& \;\; v|_{z=b_z} = b_z \gamma_{yz}^0 .$$

Notice that there are different numbers of conditions on different sides. In general, symmetry produces one condition while anti-symmetry results in two. The same applies to the subsequent shear loading cases where details of the derivation are omitted.

5.5 Under τ_{xz}^0

After considering all symmetry conditions, the boundary conditions for the unit cell subjected to this loading condition can be obtained as

$$v|_{x=0} = w|_{x=0} = 0 \quad \text{and} \quad v|_{x=b_x} = w|_{x=b_x} = 0$$

$$v|_{y=0} = 0 \quad \text{and} \quad v|_{y=b_y} = 0 \tag{26}$$

$$u|_{z=0} = v|_{z=0} = 0 \quad \text{and} \quad u|_{z=b_z} = b_z \gamma_{xz}^0 \;\; \& \;\; v|_{z=b_z} = 0 .$$

5.6 Under τ_{xy}^0

The corresponding boundary conditions are

$$v|_{x=0} = w|_{x=0} = 0 \quad \text{and} \quad v|_{x=b_x} = w|_{x=b_x} = 0$$

$$u|_{y=0} = w|_{y=0} = 0 \quad \text{and} \quad u|_{y=b_y} = b_y \gamma_{xy}^0 \;\; \& \;\; w|_{y=b_y} = 0$$

$$w|_{z=0} = 0 \quad \text{and} \quad w|_{z=b_z} = 0 . \tag{27}$$

It has been shown in this section that, using reflectional symmetries additional to translational ones, unit cells can be formulated with rather conventional boundary conditions (16) for loading in terms of microscopic stress σ_x^0, σ_y^0 or σ_z^0, (25) for τ_{yz}^0, (26) for τ_{zx}^0 and (27) for τ_{xy}^0 which do not involve equations associating the displacements on opposite sides of the unit cell. The price to pay is the fact that under different loading conditions, different boundary conditions may have to be employed. However, equation boundary conditions associated with extra d.o.f.'s will have to remain. As these extra d.o.f.'s are not really a physical part of the mesh in terms of geometry, they can be placed any where and hence should not cause any problem. Most commercial FE codes have provisions to incorporate such equation boundary conditions.

6 2-D Problems

The 3-D presentation of boundary conditions readily degenerates into 2-D problems, such as plane stress, plane strain, generalised plane strain problems and anticlastic problems. They apply to the rectangular unit cell obtained from the hexagonal layout shown in Fig. 6, as well as to the square one shown in Fig. 3. They are given as follows without detailed derivations, in the *y-z* plane, for example.

6.1 Under σ_y^0 and σ_z^0

When a 2-D unit cell, in the *y-z* plane, is subjected to macroscopic stresses σ_y^0 or σ_z^0, the boundary conditions are the same as follows

$$v|_{y=0} = 0 \quad \text{and} \quad v|_{y=b_y} = b_y \varepsilon_y^0$$

$$w|_{z=0} = 0 \quad \text{and} \quad w|_{z=b_z} = b_z \varepsilon_z^0 . \tag{28}$$

The difference between the implementations to achieve these two macroscopically uniaxial stress states is a concentrated force that needs to be imposed to the extra d.o.f. ε_y^0 or ε_z^0, respectively.

6.2 Under τ_{yz}^0

The boundary conditions for a unit cell under macroscopically uniaxial shear stress τ_{yz}^0 in the *y-z* plane are as follows

$$w|_{y=0} = 0 \quad \text{and} \quad w|_{y=b_y} = 0$$

$$v|_{z=0} = 0 \quad \text{and} \quad v|_{z=b_z} = b_z \gamma_{yz}^0 \tag{29}$$

A concentrated force at the extra d.o.f. γ_{yz}^0 delivers the macroscopically uniaxial shear stress states.

As on boundary $y=0$, displacement v is not constrained in any way and there is no restriction whether the side should remain straight after deformation. The same applies to all other sides.

6.3 Generalised plane strain problem and macroscopically uniaxial stress state σ_x^0

For generalise plane strain problems, an extra d.o.f. ε_x^0, in addition to ε_y^0, ε_z^0 and γ_{yz}^0, has to be introduced, which can be dealt with in the same manner as other extra d.o.f.'s corresponding to macroscopic strains. This extra d.o.f. should be left free when applying macroscopically uniaxial stress states σ_y^0 and σ_z^0 but constrained for τ_{yz}^0, as τ_{yz}^0 is anti-symmetric under the reflectional symmetry while ε_x^0 is symmetric. For UD composites, the generalised plane strain problem is the only 2-D formulation which is capable of achieving macroscopically effective uniaxial stress state.

6.4 Under τ_{xz}^0 and τ_{xy}^0 in an anticlastic problem

The anticlastic problem in the *y-z* plane involves only one displacement *u*. When a macroscopically uniaxial shear stress τ_{xz}^0 is applied, from Subsection 5.5, the boundary conditions for the unit cell can be obtained as

$$u\big|_{z=0}=0 \qquad \text{and} \qquad u\big|_{z=b_z}=b_z\gamma_{xz}^0 \tag{30}$$

while edges y=0 and $y=b_y$ are left free. A concentrated force can be applied to the extra d.o.f. γ_{xz}^0 to deliver a macroscopically uniaxial stress state τ_{xz}^0 and the nodal displacement at γ_{xz}^0 gives this macroscopic strain directly.

Similar arguments apply to the macro-scopically uniaxial stress state τ_{xy}^0 and from Subsection 5.6, the corresponding boundary conditions are obtained as

$$u\big|_{y=0}=0 \qquad \text{and} \qquad u\big|_{y=b_y}=b_y\gamma_{xy}^0 \tag{31}$$

while edges z=0 and $z=b_z$ are left free.

7 Deformation of the sides of unit cells

7.1 3-D unit cell for particle reinforced composites with simple cubic particle packing

A unit cell for simple cubic packing was presented in [3] and a mesh was generated with a spherical geometry for particle and appropriate constituent material properties in the examples. Only macroscopically uniaxial stress state τ_{yz}^0 is examined here. The boundary conditions are as given in (16) and (25), respectively. The von Mises stress contour plot is shown in Fig. 7. The results obtained here also agree identically with those in [3], although the corresponding contour plot was not shown in [3]. According to the boundary conditions given in (25), only the *x*-faces, i.e., x=0 and $x=b_x$, have to remain flat after deformation, while the boundary conditions on the remaining faces impose no restriction in this regard. As a result, the remaining two pairs of faces, i.e. *y*-faces and *z*-faces, do not have to remain flat. Fig.4 illustrated the curved trend for these two faces. The curvature of these faces reduces as the disparity of properties between the particle and the matrix reduces. In fact, flat faces are expected when the particle and matrix share identical properties. The same observation applies to the unit cell when it is subjected to either of the two remaining macroscopic stress states, τ_{zx}^0 and τ_{xy}^0. The only difference is that the faces remaining flat after deformation become *y*-faces and *z*-faces instead, respectively, while other faces warp after deformation, in general.

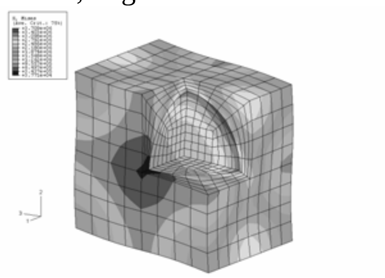
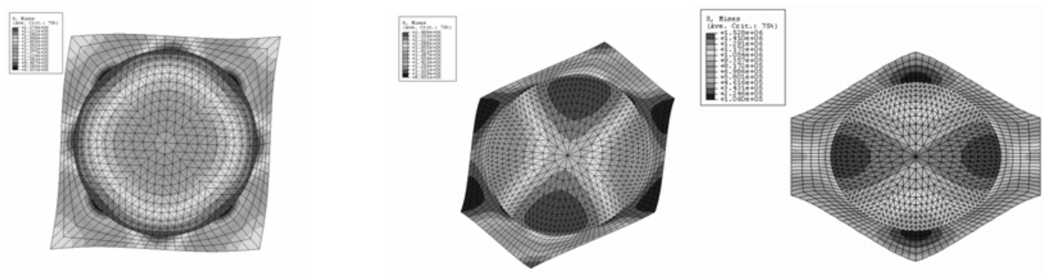


Fig 4 Deformation (simple cubic packing)

7.2 2-D unit cell for UD fibre reinforced composites with square fibre packing

Applying boundary conditions as given in Section 6 above, 2-D unit cells can be analysed pertinent to UD fibre reinforced composites with circular fibre cross-section. The examples here correspond to the cases published in [2]. As in [2], generalised plane strain conditions apply to the problem for macroscopic stress states σ_x^0, σ_y^0, σ_z^0 and τ_{yz}^0, the *x*-axis being along the fibre while the anticlastic problem for macroscopic stress states τ_{zx}^0 and τ_{xy}^0 can be analysed using heat transfer as an analogy to avoid 3-D modelling.

Once again, perfect agreement in results can be obtained between the unit cells presented here and those in [1,2] for both square packing and hexagonal packing. Similar observations to those in their 3-D counterparts of the previous subsection can be made on the deformation of the sides of the unit cells. Under direct macroscopic stress states, all the sides of a square unit cell remain straight after deformation. However, under other loading conditions or for hexagonal unit cells, sides may not remain straight after deformation as shown in Fig.8 unless the fibre has the same elastic properties as the matrix. For macroscopic stress states τ_{zx}^0 and τ_{xy}^0, the sides may look straight from the perspective along the *x*-axis (fibre direction) but the *y-z* plane itself warps into a curved surface. The sides are in fact curved in space.



(a) (b) (c)

Figure 5 Deform edges of unit cell (a) square under τ_{yz}^0 (b) hexagonal under τ_{yz}^0 (c) hexagonal under σ_y^0

8 Effects of microstructures implied by different unit cells

Assume a 2-D microstructure involving inclusions of an elliptical cross-section inclined at 30°. The ellipse is of 2:1 aspect ratio and occupies a volume fraction of 40%. The elastic properties of the inclusion and the matrix are assumed as listed in Table 1. The same mesh as shown in Fig.6 will be used for both unit cells corresponding to microstructures shown in Fig. 1 and 2, respectively.

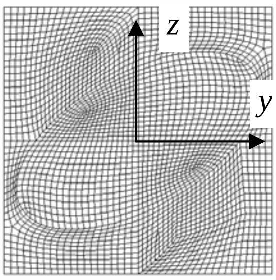


Fig. 6 Mesh (elliptical reinforcement)

Table 1 Properties of the constituents

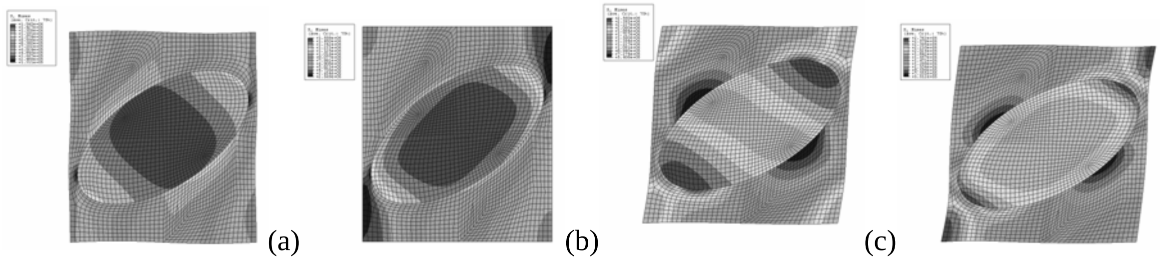
Properties	Inclusion	Matrix
E	10 GPa	1 GPa
ν	0.2	0.3

The von Mises stress contour plots at deformed configurations under macroscopic stress states σ_z^0 and τ_{yz}^0 (=1MPa) are presented and compared in Fig.7. It is obvious that differently assumed microstructures, as implied by the two different unit cells result in different stress distributions microscopically. The differences are even more pronounced when effective properties are extracted from these unit cells and compared as listed in Table 2 where properties η_{ij} are defined as the ratio of shear strain γ_j to the direct strain ε_i when the unit cell is subjected to a macroscopically uniaxial direct stress state σ_i, and μ_{ij} is the ratio of shear strain γ_j to shear strain γ_i when the unit cell is subjected to a macroscopically pure shear stress state τ_i [13]. These properties in the material's principal axis vanish for orthotropic material, as is the case for the unit cell corresponding to Fig.2c.

Table 3 Effective properties

Effective properties	Unit cell in Fig. 2b	Unit cell in Fig. 3c
E_1	4.603 GPa	4.605 GPa
E_2	2.183 GPa	2.372 GPa
E_3	1.864 GPa	1.890 GPa
G_{23}	0.6803 GPa	0.6710 GPa
G_{13}	0.7016 GPa	0.7144 GPa
G_{12}	0.9180 GPa	1.0288 GPa
ν_{23}	0.3586	0.3663
ν_{13}	0.2606	0.2612
ν_{12}	0.2436	0.2378
η_{14}	0.01377	0
η_{24}	-0.08768	0
η_{34}	-0.04289	0
μ_{56}	-0.1143	0

Material represented by the unit cell corresponding to Fig.1b is not orthotropic but monoclinic in general relative to the coordinate system as shown in Fig. 6. The differences, as illustrated here, will disappear when the ellipse is replaced by a circle but this is not a sufficient reason for ignoring the differences. When a unit cell is used, the user ought to be clear about the implications of the unit cell adopted on the microstructure of the materials, e.g. the one in Fig.1 or the one in Fig.2, which are apparently different enough from each other.



(a) (b) (c) (d)

Figure 10 Deformation and von Mises stress contour plots for theunit cell corresponding to (a) Fig. 2c under σ_z^0 (b) Fig. 3c under σ_z^0 (c) Fig. 2c under τ_{yz}^0 (d) Fig. 3c under τ_{yz}^0

8 Conclusions

Unit cells for micromechanical analyses have to be introduced with due consideration of the microstructures implied by the unit cell. Boundary conditions for unit cells representing microstructures of periodic patterns should follow entirely from the symmetries present in the microstructure represented by the unit cell, rather than from one's intuition. The symmetries include translations, reflections and rotations. Using translations alone leads to boundary conditions in the form of equations relating displacements on opposite sides of the boundary of the unit cell. Further use of reflection symmetries, if they exist, can avoid such equation boundary conditions, making the application of boundary conditions easier. However, users must be aware of the differences in the microstructures implied by the boundary conditions for the unit cell. Although unit cells may look identical geometrically, different boundary conditions imposed would associate the unit cell with rather different microstructures. It has been illustrated in this paper that such differences in the microstructures may result in rather different effective properties of the composites represented by the unit cells.

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