Sensitivity of responses of three micro-mechanics approaches to changes in unit cell configuration and inclusion shape

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\textbf{A R T I C L E   I N F O}

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Material parameters
Unit cell configuration

\textbf{A B S T R A C T}

We use three micromechanics approaches, namely, the method of cells (MoCs), the Fourier series approach (FSA) and the transformation field analysis (TFA) to delineate the sensitivity of their predictions to changes in the unit cell configuration. The three approaches are formulated to have identical final expressions relating the local sub-cell strains to the homogenized strains in the unit cell. The cubic-edge, the hexagonal close-packed and the cubic-diagonal unit cell configurations are employed to study the elasto-plastic response of a Boron-Aluminum fiber reinforced composite under transverse loading, and compare present results with Brockenbrough et al.'s findings who used the finite element method. The elasto-plastic response predicted from the cubic-edge unit-cell shows the most hardening while that from the cubic-diagonal unit-cell the least hardening. Of the three approaches employed, the elasto-plastic response predicted by the MoCs is closest to that of Brockenbrough et al. The effect of fiber cross section on the elasto-plastic response analyzed using only the TFA approach is found to be significant for both elastic constants and plastic hardening.

\textbf{1. Introduction}

Analytical micro-mechanics schemes provide an efficient means to study heterogeneous materials. It is thus important to select a scheme that adequately captures effects of the microstructure, and the distribution of constituents and their mechanical properties on inelastic deformations, damage and failure of a heterogeneous structure. Out of the many micro-mechanics schemes developed and employed to study composites, three approaches, namely, the Method of Cells (MoCs) \cite{1, 2}, the Transformation Field Analysis (TFA) \cite{3, 4} and the Fourier Series Approach (FSA) \cite{5, 6} stand out because of their general framework within which different unit cells/representative volume elements (RVEs) can be easily analyzed. The MoCs, developed by Aboudi et al. \cite{1, 2}, has been employed to study inelastic deformations of short fiber \cite{7}, long fiber \cite{20} and woven metal matrix composites \cite{8}. Matzenmiller and Gerlach \cite{9} used it to analyze fiber matrix interface debonding in viscoelastic composites. Haj-Ali and Muliana \cite{10} employed it to study the non-linear viscoelastic behavior of laminated composites. Dvorak et al. \cite{11, 12} employed the TFA to characterize the elasto-plastic response of a fiber reinforced metal matrix composite and the visco-elastic response of a glass fiber reinforced resin. Furthermore, Bahei-El-Din et al. \cite{13} used the TFA to delineate damage in woven fabric composites. Pruchnicki \cite{5} and Walker et al. \cite{6} used the FSA to study inelastic deformations in a fiber reinforced metal matrix composite. Gopinath and Batra \cite{14} employed the FSA for studying elasto-plastic deformations of off-axially loaded AS4-PEEK composite, and Wang et al. \cite{15} used it to determine the effective stiffness of periodic masonry structures.

Here, we characterize the sensitivity to changes in the unit cell configuration of the elasto-plastic response of homogenized Boron-Aluminum composites predicted by the three approaches (MoCs, TFA and FSA). As far as we can ascertain from the literature search, it has not been done. It will help identify deficiencies and advantages of each approach and will allow one to make a more informed choice of adopting an appropriate approach. The sensitivity study is carried out by analyzing the elasto-plastic deformations of a fiber reinforced composite using the cubic-edge, the cubic-diagonal and the hexagonal close-packed configurations depicted in Fig. 1. For a given volume fraction of fibers in a composite it is not readily apparent if the choice of a unit cell will influence the predicted response. However, the analysis, by the finite element method (FEM), of deformations of unit cells of fiber reinforced composites by Zhu and Sun \cite{16}, Brockenbrough et al.
Sensitivity of responses of three micro-mechanics approaches to changes in unit cell configuration and inclusion shape

Table 1
Elastic constants for Aluminum matrix and Boron fibers.

<table>
<thead>
<tr>
<th></th>
<th>Aluminum 6061-O</th>
<th>Boron</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>69 GPa</td>
<td>410 GPa</td>
</tr>
<tr>
<td>ν_{12}</td>
<td>0.33</td>
<td>0.2</td>
</tr>
</tbody>
</table>

[17] and Brockenbrough and Suresh [18] have shown that under transverse loading the cubic edge (i.e., square packing) arrangement of fibers gives the most hardening after initial yield while the cubic diagonal arrangement the least hardening. Brockenbrough et al. and Ye et al. [29] noticed that fiber shapes influenced the hardening behavior, with square fibers exhibiting more hardening than circular ones. Arnold et al. [19] have reviewed the literature on the influence of the fiber shape and distribution on the elastic and the inelastic response of metal matrix composites. Love and Batra [37] used the FEM to analyze transient deformations of tungsten particulates embedded in a Nickel-Iron matrix and deduced thermo-elasto-visco-plastic properties of the homogenized material by modeling each constituent and the mixture by the Johnson-Cook relation. Jiang and Batra [38-40] employed micromechanical approaches to ascertain properties of a homogenized material. Hassan and Batra [41] used the mechanics of material approach for homogenizing a unidirectional fiber-reinforced composite. Nemat Nasser and Hori [30] and Charalambakis [42] have reviewed various micro-mechanical theories.

As noted in [17] experimental results for transverse loading exhibit scatter beyond the proportionality limit primarily because of issues with gripping and difficulty in applying uniform loads over the gauge length. Under such circumstances it would be helpful to explore the use of micromechanics approaches to complement experiments. Results from the current analysis are compared with those of Brockenbrough et al. [17]. We have not scrutinized the effect of fiber cross-section using either the MoGs or the FSA as a sub-cell since these methods must have a rectangular cross section; thus, only the TFA approach is used for this.

The remainder of the paper is organized as follows. In Section 2 we briefly review the three micromechanics approaches and present their final micro-mechanical expressions in the same format along with their implementation within a FE scheme. Predictions from the three approaches for elasto-plastic deformations of a Boron-Aluminum composite are compared in Section 3. We discuss results and summarize conclusions in Section 4.

2. Brief review of the three micromechanics approaches

Gopinath and Batra [14] have recently proposed a common framework for the three approaches. Thus, these are only briefly reviewed here for completeness. Consider a unit-cell/RVE sub-divided into N sub-cells. The homogenized macrostrain, ε, corresponding to infinitesimal deformations is given by a volume average of the local strains, ε_{r}, within the sub-cells in which strains are assumed to be uniform. That is,

\[ \varepsilon = \sum_{r=1}^{N} c_{r} \varepsilon_{r} \]  

where c_{r} is the volume fraction of the sub-cell r.

Using constitutive relations, we relate \varepsilon_{r} in sub-cell r to \varepsilon by [4]

\[ \varepsilon_{r} = A_{s} \varepsilon + \sum_{r=1}^{N} D_{m} \mu_{r} \]  

where \mu_{r} is the transformation strain and includes all inelastic strains, A_{s} is the strain concentration tensor, and D_{m} is strain transformation tensor.

All three micro-mechanics approaches can be formulated to appear as Eq. (2).

2.1. Method of cells approach

We identify sub-cells by the symbol β = 10\delta_{i}, in the vertical direction, and by γ = 10\gamma_{j}, in the horizontal direction. The cross-sectional dimensions of the unit cell are L_{x}L_{y}L_{z}, and each cell has cross-sectional dimensions H_{x}H_{y}H_{z}. Using strain-displacement relations and the interface displacement continuity conditions, we arrive at the following expressions connecting strains in a sub-cell to the homogenized strain [1,2].

\[ \varepsilon_{i}^{(\beta)} = \delta_{i} \quad \sum_{\gamma=1}^{N} H_{\gamma} \varepsilon_{\gamma}^{(\beta)} = H_{\beta} \sum_{\gamma=1}^{N} L_{\gamma} \varepsilon_{\gamma}^{(\beta)} = L_{\beta} \sum_{\gamma=1}^{N} M_{\gamma} \varepsilon_{\gamma}^{(\beta)} = M_{\beta} \sum_{\gamma=1}^{N} \sum_{\delta=1}^{N} H_{\gamma} L_{\delta} M_{\beta} \varepsilon_{\gamma}^{(\beta)} = L_{\beta} H_{\beta} M_{\beta} \]  

We write Eq. (3) in matrix form as
Table 2
Voce hardening parameters for Aluminum 6061-O.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k ) (yield stress)</td>
<td>43 MPa</td>
</tr>
<tr>
<td>( R )</td>
<td>30 MPa</td>
</tr>
<tr>
<td>( R )</td>
<td>72 MPa</td>
</tr>
<tr>
<td>( \delta )</td>
<td>35</td>
</tr>
</tbody>
</table>

\( \mathbf{A}_0 \mathbf{d}_0 = \mathbf{J} \varepsilon \)  

where \( \varepsilon_0 \) and \( \varepsilon \), respectively, represent the sub-cell and the homogenized strains.

Since the number of unknowns in Eq. (4) exceeds the number of equations, these are supplemented with the following traction continuity conditions across interfaces of sub-cells where we have used constitutive equations, additive decomposition of infinitesimal strains into elastic and plastic parts, and designated plastic strains by a superscript \( p \).

\( \mathbf{A}_0 (\varepsilon_0 - \varepsilon_0^p) = 0 \)

Combining Eq. (4) and Eq. (5) we get

\[
\begin{bmatrix}
\mathbf{A}_0 \\
\mathbf{A}_G
\end{bmatrix} \mathbf{d}_0 = \begin{bmatrix}
0 \\
\mathbf{J}
\end{bmatrix} \varepsilon + \begin{bmatrix}
\mathbf{A}_0 \\
\mathbf{A}_G
\end{bmatrix} \varepsilon_0^p
\]

which we rewrite as

\( \varepsilon_0 = [\mathbf{A}^{\text{Mac}}] \varepsilon + [\mathbf{D}^{\text{Mac}}] \varepsilon_0^p \)

In Eq. (7),

\[
[\mathbf{A}^{\text{Mac}}] = \begin{bmatrix}
\mathbf{A}_0^{-1} & 0 \\
\mathbf{A}_G & 1
\end{bmatrix}
\]

\[
[\mathbf{D}^{\text{Mac}}] = \begin{bmatrix}
\mathbf{A}_0^{-1} & \mathbf{A}_G \\
0 & 0
\end{bmatrix}
\]

are, respectively, the strain concentration matrix, and the transformation strain matrix for the plastic strain.

2.2. Fourier series approach

Following Walker et al. [6] we define eigen-strain, \( \varepsilon_0^p \), by

\[
C^{\text{Mac}}_{ijkl} \varepsilon_0^p = C^{\text{Mac}}_{ijkl} (\varepsilon_0 - \varepsilon_0^p) - \delta C^{\text{Mac}}_{ijkl} (\varepsilon_0^p + \varepsilon_0 - \varepsilon_0^p)
\]

where \( \delta C^{\text{Mac}}_{ijkl} = \theta (C^{\text{Mac}}_{ijkl} - C^{\text{Mac}}_{ijkl}) \), \( \theta = 1 \) corresponds to the fiber and \( \theta = 0 \) to the matrix.

Assuming periodicity of the micro-structure in the composite, the displacement field \( u \) and the eigen-strain \( \varepsilon \) are expressed as Fourier series. Using constitutive and equilibrium equations, we write the average strain in the \( g \)-th sub-cell as [6]

\[
\varepsilon_0^p = \sum_{g=1}^{G} \left[ f^T \varepsilon_0^p \right] \varepsilon_{g} - \sum_{g=1}^{G} \left[ f^T \varepsilon_0^p \right] s_{g}^p
\]

where

\[
C^{\text{Mac}}_{ijkl} = \sum_{g=1}^{G} \sum_{i=6}^{12} \sum_{j=6}^{12} (\mathbf{M}_i \mathbf{M}_j \mathbf{Q}^i \mathbf{Q}^j (\xi)) \mathbf{Q}^i \mathbf{Q}^j (\xi), \quad \text{and} \quad \sum_{g=1}^{G} \sum_{i=6}^{12} \sum_{j=6}^{12} s_{g}^p
\]

\[
Q^i (\xi) = \frac{1}{V} \int_{V} \exp (i \mathbf{q} \cdot \mathbf{x}) dV (\mathbf{x}), \quad \text{and} \quad \text{volume fraction} \ \beta = \frac{V_e}{V}
\]

Other notations are explained in [14] wherein Eq. (9) is written as

\[
\varepsilon^T = [\mathbf{A}^{TT}] \varepsilon^p + [\mathbf{D}^{TT}] \varepsilon_0^p
\]

with the strain concentration and the strain transformation matrices, \([\mathbf{A}^{TT}] \) and \([\mathbf{D}^{TT}] \), having the following expressions.

\[
[\mathbf{A}^{TT}] = \begin{bmatrix}
\sum_{g=1}^{G} \mathbf{M}^g \\
\vdots \\
\sum_{g=1}^{G} \mathbf{M}^{g-1}
\end{bmatrix}
\]

\[
[\mathbf{D}^{TT}] = \begin{bmatrix}
\mathbf{M}^1 & \mathbf{M}^2 & \cdots & \mathbf{M}^N \\
\vdots & \vdots & \ddots & \vdots \\
\mathbf{M}^{N-1} & \mathbf{M}^N & \cdots & \mathbf{M}^{N-1}
\end{bmatrix}
\]
Table 3
Comparison of elastic constants for 46% volume fraction of Boron fiber-reinforced Aluminum matrix predicted by different techniques.

<table>
<thead>
<tr>
<th></th>
<th>$E_t$ (GPa)</th>
<th>$v_t$</th>
<th>$E_r$ (GPa)</th>
<th>$G_r$ (GPa)</th>
<th>$G_t$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic edge</td>
<td>Expt.</td>
<td>228</td>
<td>0.24</td>
<td>138</td>
<td>57</td>
</tr>
<tr>
<td></td>
<td>M.T</td>
<td>226</td>
<td>0.264</td>
<td>134</td>
<td>53</td>
</tr>
<tr>
<td></td>
<td>FEM</td>
<td>228</td>
<td>0.286</td>
<td>153</td>
<td>60</td>
</tr>
<tr>
<td></td>
<td>MoCo</td>
<td>226</td>
<td>0.265</td>
<td>146</td>
<td>43</td>
</tr>
<tr>
<td></td>
<td>PSA</td>
<td>226</td>
<td>0.263</td>
<td>151</td>
<td>44</td>
</tr>
<tr>
<td></td>
<td>TFA</td>
<td>226</td>
<td>0.263</td>
<td>153</td>
<td>44</td>
</tr>
<tr>
<td>Hexagonal close packed</td>
<td>FEM</td>
<td>228</td>
<td>0.263</td>
<td>138</td>
<td>51</td>
</tr>
<tr>
<td></td>
<td>MoCo</td>
<td>226</td>
<td>0.27</td>
<td>136</td>
<td>43</td>
</tr>
<tr>
<td></td>
<td>PSA</td>
<td>226</td>
<td>0.261</td>
<td>143</td>
<td>48</td>
</tr>
<tr>
<td></td>
<td>TFA</td>
<td>226</td>
<td>0.265</td>
<td>145</td>
<td>49</td>
</tr>
<tr>
<td>Cubic Diagonal</td>
<td>FEM</td>
<td>227</td>
<td>0.262</td>
<td>134</td>
<td>48</td>
</tr>
<tr>
<td></td>
<td>MoCo</td>
<td>226</td>
<td>0.27</td>
<td>121</td>
<td>43</td>
</tr>
<tr>
<td></td>
<td>PSA</td>
<td>226</td>
<td>0.263</td>
<td>128</td>
<td>55</td>
</tr>
<tr>
<td></td>
<td>TFA</td>
<td>226</td>
<td>0.259</td>
<td>135</td>
<td>59</td>
</tr>
</tbody>
</table>

Figure 3. Axial stress vs axial strain curves for Aluminum 6061-O.

2.3. Transformation field analysis approach

In the TFA the concentration and the strain transformation tensors are numerically determined by using the FEM. Miehe and Koch [21] have demonstrated that applying periodic boundary conditions readily satisfies Hill’s averaging theorem (i.e., the microscopic work must equal the macroscopic work) and better estimates homogenized properties than those predicted by applying constant tractions or displacements that also satisfy Hill’s theorem. For periodic boundary conditions each node pair $q$ on a boundary surface of the RVE must satisfy the constraint Eq. (11).

$$u(x^*) - u(x^*)_q = \varepsilon(x^* - x^*)_q = \begin{bmatrix} \varepsilon_{x} \varepsilon_{y} \varepsilon_{z} \\ \varepsilon_{xy} \varepsilon_{y} \varepsilon_{z} \\ \varepsilon_{xz} \varepsilon_{zy} \varepsilon_{z} \end{bmatrix} \begin{bmatrix} x^* - x^* \\ y^* - y^* \\ z^* - z^* \end{bmatrix}_q$$

These conditions in terms of the macro-strain $\varepsilon$ can be enforced either through Lagrange multipliers [21,22] or tie constraints [22–24]; we adopt the latter. Assuming that the domain is free of eigenstrains, i.e., $\varepsilon_0 = 0$ in Eq. (2), we find the strain concentration tensor $A_s$ from $e_s = A_{st}$ by applying periodic boundary conditions using macro-strain components of unit magnitude individually. We similarly determine the eigenstrain transformation tensors $D_{tr}$ by applying unit eigen-strain component in one element of the FE mesh. For a unit cell discretized into N elements, 6 N load cases are considered to evaluate $D_{tr}$ [12].

2.4. Effective stiffness of the RVE

We follow Dvorak [25] for determining the stiffness matrix, $C^{RVE}$, of the RVE for elasto-plastic deformations, and the following constitutive equation for the $\alpha$ sub-cell

$$\sigma^{\alpha} = C^{\alpha} : \varepsilon^{\alpha} + \sigma^{\alpha^0} \varepsilon^{\alpha}$$

where $C^{\alpha}$ is the relaxation stress, and $C^{\alpha^0}$ the plastic modulus. Substitution for $\varepsilon^{\alpha}$ in the expression for $\sigma^{\alpha}$ gives

$$\sigma^{\alpha^0} = -C^{\alpha} : \varepsilon^{\alpha^0}$$

Using Eq. (2) we write local strains in the ‘$\alpha$’ sub-cell as
**Fig. 4.** Comparison of the transverse normal stress vs. the transverse axial strain from the MoCs and the FEM assuming square fibers.

**Fig. 5.** Comparison of the transverse normal stress vs. the transverse axial strain from the FSA and the FEM assuming square fibers.

\[ \varepsilon^a = A^a : \varepsilon_{\text{RVE}} + \sum_{\beta=1}^{N} D^{\alpha\beta} : \varepsilon^\beta \]

Substituting \( \varepsilon^{\text{RVE}} = -S^a : \varepsilon^a \), \( \sigma^{\text{RVE}} = C^{\alpha\beta} : \varepsilon^\beta \) and rearranging the expression we get

\[ \varepsilon^{\text{RVE}} = \left( I + \sum_{\beta=1}^{N} D^{\alpha\beta} : S^\beta : C^{\alpha\beta} \right)^{-1} : A^a : \varepsilon_{\text{RVE}} = A^a : \varepsilon_{\text{RVE}} \]

(13)

Thus

\[ C_{\text{RVE}} = \sum_{\alpha=1}^{N} f^a C^\alpha : A^\alpha \]

(14)

For inelastic deformations the concentration tensor \( A^a \) replaces \( A^\alpha \), and the elastic-plastic stiffness matrix replaces the elastic stiffness matrix in Eq. (14). Note that for elastic deformations, \( A^a = A^\alpha \).

After determining strains in sub-cells, stresses in the RVE are calculated by volume averaging them over the sub-cells, i.e.,

\[ \sigma_{\text{RVE}} = \sum_{\alpha=1}^{N} f^a \sigma^\alpha \]

(15)

### 2.5. Implementation of micro-mechanics approaches within a FE scheme

The above-mentioned three micromechanics approaches are
implemented in a nonlinear FE program that uses the Newton-Raphson method to solve for nodal displacements. The strain concentration and the strain transformation matrices given in Eq. (2), determined from a micromechanics approach, are stored in the database and are called upon to calculate strains and the stiffness matrix (elastic for fibers and elastic-plastic for the matrix) iteratively within the unit cell. The elemental stiffness matrix and the internal force required for the Newton-Raphson method for global convergence are, respectively, determined using Eqs. (14) and (15). We note that strains at Gauss points represent the homogenized/average strain within the unit cell. Additional details of the implementation are given in [14].

3. Results

3.1. Material parameters

Elastic constants for the Aluminum matrix and the Boron fibers used by Brockenbrough et al. [17] are listed in Table 1. We assume the Aluminum and the Boron fibers to, respectively, deform elastplastically and elastically. The von Mises yield criteria and the associative flow rule govern plastic deformation of the Aluminum. The Voce hardening law

$$K(\alpha) = k + (R_0)\alpha + R[1 - \exp(-\delta\alpha)]$$  \hspace{1cm} (16)

commonly employed in metal plasticity and more specifically for the Aluminum is used for plastic deformations [26,28]. In Eq. (16), $\alpha$ is the effective plastic strain, $k$ the yield stress, $R_0$ the slope of the asymptotic straight line to the effective stress-effective plastic strain curve, $R$ the difference in the value between the intercept to the effective stress axis ($y$-axis) of the asymptotic straight line and the yield stress and $\delta$ accounts for the curvature of the curve. These variables are depicted in Fig. 2, and are described in [28]. The nonlinear elasto-plastic equations are numerically solved by using the implicit Newton-Raphson method; details are provided in Appendix-1 [27]. The values of hardening parameters, listed in Table 2, were found by following the approach described in [14]. It is clear from the computed effective stress vs. the effective plastic strain curve and the one from the test data, exhibited in Fig. 3, that the two curves are very close to each other.

3.2. Estimation of elastic constants

For three unit cell configurations corresponding to 46% volume fraction of square cross-section Boron fibers, we have compared in Table 3 values of elastic constants predicted from the three micromechanics approaches with their experimental values reported by Becker et al. [19], the FEM predictions of Brockenbrough et al. [17], and those computed using the Mori-Tanaka (M-T) scheme. The subscripts ‘L’ and ‘T’, respectively, stand for the longitudinal (along the fibers) and the transverse directions. We recall that the effect of the unit cell configuration is not captured by the M-T scheme, thus the longitudinal moduli and Poisson's ratio are unaffected by the unit cell configuration. However, the transverse elastic modulus and the shear moduli show sensitivity to the unit-cell configuration. For the HCP configuration there is less than 1% difference in the predicted values of the elastic moduli in the two transverse directions, and the average value is reported here.

3.3. Elasto-plastic response under transverse loading

In Figs. 4–6, we compare the response of the composite to transverse normal loading by using the MoCs, the FSA and the TFA with the FEM.
Table 4
Effect of fiber geometry on predicted values of elastic constants.

<table>
<thead>
<tr>
<th></th>
<th>$E_1$ (GPa)</th>
<th>$v_{12}$</th>
<th>$E_2$ (GPa)</th>
<th>$G_{12}$ (GPa)</th>
<th>$G_{13}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic edge</td>
<td>228</td>
<td>0.263</td>
<td>152</td>
<td>57</td>
<td></td>
</tr>
<tr>
<td>TFA-Square</td>
<td>226</td>
<td>0.263</td>
<td>153</td>
<td>44</td>
<td>54</td>
</tr>
<tr>
<td>TFA-Hexagon</td>
<td>226</td>
<td>0.263</td>
<td>150</td>
<td>45</td>
<td>54</td>
</tr>
<tr>
<td>TFA-Octagon</td>
<td>226</td>
<td>0.263</td>
<td>149</td>
<td>45</td>
<td>53</td>
</tr>
<tr>
<td>Hexagonal close packed</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>TFA-Square</td>
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<td>0.262</td>
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<td>50</td>
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<td>TFA-Hexagon</td>
<td>226</td>
<td>0.265</td>
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<td>53</td>
</tr>
</tbody>
</table>

Fig. 8. Effect of inclusion shape on composite's inelastic response under transverse loading using the TFA approach.

The results of Brockenbrough et al. for fibers of square cross-section. All micromechanics approaches show sensitivity to the change in configuration, with the cubic edge (cubic diagonal) packing exhibiting the most (the least) hardening after yield. The elasto-plastic response predicted from the MoC's approach is closest to that from the FEM. The responses from the TFA and the FSA approaches are much stiffer.

3.4. Effect of fiber shape on the elasto-plastic response

Fibers in a composite are rarely of uniform cross-section. It is common to approximate their shapes as circular and square in micromechanics theories. Results presented in sub-sections 3.2–3.4 assume the fiber cross-section to be a square that imposes certain constraints. For example, square cross-section fibers cannot be used when the volume fraction exceeds 50% for the cubic diagonal arrangement. It is inherently difficult to study the effect of fiber shape using the MoCs and the FSA as it entails approximating the geometry by cuboidal unit cells which follow curved contours of the inclusions. Thus, the effect of shape is studied using only the TFA as it is relatively simple to capture geometric changes with a FE mesh. Fig. 7 shows three cross-sections studied in which the shape of a fiber transitions from a square to an octagon. We note that results with decagon fibers are similar to those with octagonal fibers and are not included here. The number of FEs used to capture various fiber shapes ranged between 420 and 480, the effect of the FE mesh refinement on the elasto-plastic response is discussed in Section 3.5. We note that the maximum difference of 4% was observed in the transverse elastic modulus for cubic diagonal arrangement for different FE mesh sizes considered, and the modulus decreased with an increase in the number of FEs. In Table 4 we have listed values of elastic constants predicted from the TFA approach for the three fiber shapes and also those reported by Brockenbrough et al. for circular fibers. It is clear that the transverse elastic modulus and the two shear moduli are sensitive to the fiber shape primarily for the cubic diagonal arrangement and relatively insensitive to the cubic edge and the hexagonal close packing arrangements.

In Fig. 8 we have compared the inelastic response for the four fiber shapes for each of the three unit cell configurations under transverse loading. The cubic-edge (cubic-diagonal) fiber arrangement shows the stiffest (softest) response, and the hexagonal packing arrangement falls in-between the two. Comparing the response for the fiber shapes, we see that square (octagonal) fibers show the stiffest (softest) response for all fiber arrangements. The cubic diagonal arrangement is most sensitive to changes in the fiber shape. Unlike predictions for the square fibers, predictions for the octagonal fibers are comparable to those from the FE approach for circular fibers.

The sensitivity of the elasto-plastic response to the fiber geometry and packing arrangements can be explained in terms of the packing efficiency. A possibility is that more fibers are present within a given volume then more load can be transferred between the fiber and the matrix resulting in increased plastic deformation within the matrix unless fibers start touching each other. We note that circular fibers have the highest packing efficiency, hence more the shape deviates from being circular the lower would be the packing efficiency. The shape factors, perimeter of cross-section/perimeter of circular cross-section, for square, hexagonal and octagonal fibers equal, respectively, 1.13, 1.05 and 1.027. The packing factor for the cubic-edge, the HCP and the cubic-diagonal arrangements are, respectively, $\pi/2.2\pi/\sqrt{3}$ and $[36]$. Naaman [31] and Xu et al. [32] have also used the shape factor to explain differences in the strength of fiber-reinforced composites with fibers of different shapes. Romansova et al. [33] used the shape factor to characterize roughness of reinforcing particles and study its influence on the failure of Aluminum reinforced particulate composites. This argument, though simple, does not give a true understanding of the geometric constraints imposed by the relatively rigid fibers on the
plastic flow of the matrix; this is better understood by looking at the local plastic strains and the hydrostatic stress. Studies on metal matrix composites that have ascribed hydrostatic stress buildup to failure and used it to interpret inelastic response of fiber reinforced composites include [17,34,35].

Figs. 9 and 10 depict, respectively, for a macro-strain of 0.6%, contour plots of the effective plastic strain and of the hydrostatic stress in a unit-cell for cubic-edge and cubic-diagonal arrangements. Plots were generated using MATLAB’s grid-data interpolation function using field variables at centroids of the sub-cell locations. White border lines indicate fiber location within the unit cell. The imposed periodic boundary conditions and the symmetric arrangement of fibers within the unit cell about the XY- and the XZ- planes (the X-axis is along the fibers) result in symmetric contour plots of the field variables about these planes. As has been previously reported by others, e.g., see [17,35], we find that magnitudes of the local strains and stresses are much higher than their respective values in the homogenized material. From the contour plots we see that for the cubic-edge arrangement magnitudes of the effective plastic strain increase as we go from the square to the octagonal fibers. This can be attributed to the buildup of the hydrostatic stress along surfaces of the fibers which limits the plastic flow of material. The area of buildup of the hydrostatic stress in the matrix is proportional to the circumference of the fiber and is thus highest (least) for square (octagonal) fibers. The magnitude of the hydrostatic stress is slightly more for hexagonal fibers than that for square and octagonal fibers that have nearly the same value. It is interesting to note that there is no concentration of plastic strains at the corners of the fiber geometry as one would have expected possibly due to a lack of...
interaction with other fibers in the cubic-edge unit cell. For cubic diagonal arrangement which shows plastic strain concentration at 46% fiber volume fraction for square fibers disappears at 23% fiber volume fraction; e.g., see contour plots in Fig. 13b for the lower fiber volume concentration. For the cubic-diagonal arrangement magnitudes of the effective plastic strains are comparable to each other and we find high plastic strains concentrated along corners of the fiber geometry. The regions of high plastic strains are more for square fibers followed by those for hexagonal and then for octagonal fibers. We note that there is no concentration of plastic strains at the corners of the octagonal fibers as it does for the square and the hexagonal fibers. This is primarily attributed to the increase in the interior angle of the polygon (90° for square, 120° for hexagon and 135° for octagon) that reduces the stress concentration at the corners. The interaction among fibers within a unit cell also plays a role in the buildup of high plastic strains. The shortest distance between corners of fibers is least for the square fibers followed by that for the octagonal and the hexagonal fibers. From the contour plots we also observe that the magnitude of the hydrostatic stress is least for the octagonal fibers and the maximum for the square fibers. From these results the following three clear differences emerge when one compares the cubic-edge and the cubic-diagonal fiber arrangements. (1) For the cubic-diagonal arrangement there exist regions of high plastic zones along corners of fiber edges which are absent for the cubic-edge arrangement; this is ascribed to the interaction between fibers and the stress concentration due to the fiber geometry. (2) The buildup of the hydrostatic stress along the edges/faces of fiber cells is
much less for the cubic-diagonal arrangement than that for the cubic-edge arrangement. (3) Magnitudes of the effective plastic strains (the hydrostatic stress) are higher (lower) for the cubic-diagonal arrangement as compared to those for the cubic-edge arrangement. The geometric constraints imposed by the relatively stiff fibers in terms of the buildup of the hydrostatic stress and the plastic flow of the matrix help explain why the cubic-diagonal arrangement with the octagonal fibers shows much softer response than the cubic-edge arrangement with square fibers.

From contour plots of the field variables it appears that the development of high plastic zones at the fiber corners in the cubic diagonal arrangement is due to the interaction among fibers in the unit cell. We note that only one fiber is considered for the cubic-edge arrangement while there are five fibers within the unit cell for the cubic-diagonal arrangement. To see if including more fibers in the cubic-edge arrangement would affect the distribution of the effective plastic strain we consider configuration-2 with a fiber located at each corner of the unit cell as shown in Fig. 11a. The transverse axial stress-axial strain curve for configuration-2 (not included here) is identical to that for configuration-1. Also, from contour plots for the two configurations shown in Fig. 11b the presence of other fibers in the arrangement does not cause zones of high plastic strains to develop at the corners and the contour plots are almost identical; small differences are due to approximation errors while interpolating in MATLAB.
3.5. Mesh sensitivity study

The elasto-plastic response for transverse loading is primarily governed by the plastic deformation of the matrix. To ensure that the response is not influenced by the FE mesh all configurations were discretized with a similar mesh having 420 to 480 elements. The convergence of the solution was verified by considering the elasto-plastic response for the three configurations with square fibers, and is shown in Fig. 12. For the cubic edge configuration, no change in response was observed when the number of FEs was increased from 168 to 480. For the cubic-diagonal arrangement, the response did not noticeably change with an increase in the number of FEs from 250 to 480. However, with a FE mesh of 140 elements the response was stiffer than that for 250 FEs. For the HCP configuration the response was similar for 320 and 448 FEs but showed slightly higher stiffness with 180 FEs. Thus, the cubic-diagonal and the HCP arrangements are more sensitive to transverse loading than the cubic-edge arrangement, and the FE mesh having more than 400 FEs gives a converged response for each configuration.

3.6. Effect of volume fraction and shape of the fiber on the elasto-plastic response

Fig. 13a, b (Fig. 14a, b) shows the elasto-plastic response for loading in the transverse direction and the corresponding fringe plots of the effective plastic strain at a macro-strain of 0.6% for the composite having fiber volume fraction of 23% (11.5%) which is one-half (1/4th) the volume fraction studied by Brockenbrough et al. [17]. Only extreme cases of the cubic-edge and the cubic-diagonal unit cell configurations with square and octagonal shaped fibers are considered. We observe that at low volume fraction of fibers, there is a little influence of the unit cell configuration and the fiber shape on the inelastic response. Also, plastic strains which were concentrated near corners of the square fibers at 46% volume fraction (e.g., see Fig. 10) are now absent, confirming the importance of fiber-fiber interaction within the unit cell along with the fiber geometry. The distribution of the plastic strain also appears to be similar for the square and the octagonal fiber geometries for the two configurations at low volume fractions of fibers.

4. Conclusions

We have determined the elasto-plastic response of a fiber-reinforced composite from three micro-mechanics approaches (the Method of Cells (MoCs), the Transformation Field Analysis (TFA), and the Fourier Series Approach (FSA)) and for three unit cell configurations, namely, the cubic-edge, the cubic-diagonal and the hexagonal close-packed. The cubic-edge unit-cell shows the most hardening while the cubic-diagonal arrangement the least. Of the three approaches analyzed, the elasto-plastic response from the MoCs is comparable to that from the analysis of deformations of the unit cell by the finite element method (FEM). The FSA and the TFA yield overly stiff response as compared to that from the FEM. The effect of the fiber geometry, studied using the TFA, showed that values of the transverse elastic constants and the transverse elasto-plastic response are very sensitive to the fiber geometry. A detailed analysis of distributions of the local effective plastic strain and the hydrostatic stress indicates that not only the fiber geometry but also the interaction amongst adjacent fibers within a unit cell plays an important role in constraining the plastic flow of the matrix around the fiber. We also found that at low fiber concentrations, the fiber geometry and the choice of the unit cell become less important.

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Fig. 13. a, b. Transverse normal stress vs. transverse axial strain curve & contour plots of effective plastic strain at fiber volume fraction of 23%.
Fig. 14. a, b. Transverse normal stress vs. transverse axial strain curve & contour plots of effective plastic strains at fiber volume fraction of 11.5%.
Appendix 1. Implementation of the elasto-plastic constitutive equation: Voce hardening

The elasto-plastic deformations are analyzed by using the radial return method. In equations given below subscripts n and (n + 1) stand for the nth and the (n + 1)th time (or load) step.

The yield function is given by $f = \|\mathbf{S}\| - \frac{1}{3}K(\mathbf{a})$

where

$\mathbf{S} = \sigma - \frac{1}{3}\sigma_{ii}\delta_{ij}$ is the deviatoric stress

Evolution equations for the plastic strain (flow rule) and for $\sigma$ are assumed to be

$\dot{\epsilon}^p = \gamma n$ and $\dot{\sigma} = \sqrt{3} \gamma$

where $n = \frac{s}{\sqrt{3} \gamma}$ is the normal to the yield surface.

Eq. (17b,c) is written as

$\mathbf{e}^{p}_{n+1} = \mathbf{e}^p_n + \Delta\gamma n_{n+1} + \Delta\gamma n_{n+1,\text{total}} + \Delta\gamma n_{n+1,\text{boundary}}$

where $\Delta\gamma$ is the yield stress, and

$\mathbf{a}_{n+1} = \mathbf{a}_n + \frac{\sqrt{3}}{2} \Delta\gamma$ with $\mathbf{a}_{n+1,\text{boundary}} = \mathbf{a}_n$

$\mathbf{a}_{n+1} = \mathbf{a}_{n+1,\text{total}} + \frac{\sqrt{3}}{2} \Delta\gamma$

We write the constitutive equation as

$\mathbf{S}_{n+1} = 2\mu(\mathbf{e}_{n+1} - \mathbf{e}_n^p)$ and $\mathbf{S}_{n+1,\text{total}} = 2\mu(\mathbf{e}_{n+1} - \mathbf{e}_n^p)$ \Rightarrow $\mathbf{S}_{n+1} = \mathbf{S}_{n+1,\text{total}} = 2\mu(\mathbf{e}_{n+1} - \mathbf{e}_n^p)$

where $\mu$ is the shear modulus.

Using Eqs. (17) and (18) we get a nonlinear equation in $\Delta\gamma$ that is iteratively solved by using the Newton-Raphson method. That is,

$g(\Delta\gamma^{\text{iter}}) = \|\mathbf{S}_{n+1,\text{total}}\| - \frac{1}{3}K(\mathbf{a}^{\text{iter}}_{n+1}) - \Delta\gamma^{\text{iter}}\Delta\mu$

$Dg(\Delta\gamma^{\text{iter}}) = \frac{\sqrt{3}}{2} DK(\mathbf{a}^{\text{iter}}_{n+1}) \frac{\partial g}{\partial \Delta\gamma^{\text{iter}}} = -2 \Delta\mu$

The iteration is started assuming $\Delta\gamma^{\text{iter}} = 0$ and $\mathbf{a}^{\text{iter}}_{n+1} = \mathbf{a}_n$ with the update given by Eq. (20).

$\Delta\gamma^{\text{iter+1}} = \Delta\gamma^{\text{iter}} - \frac{g(\Delta\gamma^{\text{iter}})}{\frac{\partial g}{\partial \Delta\gamma^{\text{iter}}}}$ and $\mathbf{a}^{\text{iter+1}}_{n+1} = \mathbf{a}_n + \frac{\sqrt{3}}{2} \Delta\gamma^{\text{iter+1}}$

References


