Homogenization of Mechanical Properties of Unidirectional Fibre Reinforced Composites with Matrix and Interface Defects: A Finite Element Approach

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Abstract. Fiber Reinforced Composites find increasing applications in the areas of Aerospace, Military Armours, Bullet-proof vests, etc. As the composites are composed of two different constituents, there arises a need to determine the effective properties of the homogenous composites. Experimental determination of the effective properties is very expensive considering the amount of experiments that are required to be conducted, the time and cost to be incurred for each experiment, and the permutations and combinations of the optimal fiber volume fraction. The effective properties are essential for modeling of composites with reference to real-time applications. The micro-mechanics approach reduces most of the above mentioned complexities and helps in accurately evaluating the effective properties. In the presented paper, the properties like Young’s Modulus, Poisson Ratio, and Shear modulus of a healthy (defect free) composite is obtained by modeling a Representative Volume Element (RVE) using the commercial Finite Element Analysis (FEA) solver – Abaqus, with application of Periodic Boundary Conditions (PBC). The presented research focuses on Fiber-Reinforced Metal-Matrix composites like AA2024-Al₂O₃ and the Ceramic-Matrix composites like ZrB₂-SiC. In general, defects in composites arise during the manufacturing process. Matrix Crack, Interfacial De-bonding and Fiber Crack are the major defects which degrade the mechanical properties of composites. This paper presents the modeling of Interfacial de-bonding using the Cohesive-Zone Modelling (CZM) technique for every 90° variation in the fiber-matrix interface and the subsequent evaluation of the corresponding homogenous properties. Matrix Crack is modelled as a matrix defect with a ‘V’ notch for varying a/w ratios. For every variation in matrix crack, the corresponding properties are estimated. Numerical evaluation of the individual effects of interfacial de-bonding and fully grown matrix cracks are followed by the modelling of the coupled effects.

1. Introduction

Composite Materials have been used extensively due to their high strength along the fiber direction and high strength-to-weight ratio. Fiber-Reinforced Metal-Matrix and Ceramic Matrix Composites find tremendous applications specifically in automotive, aerospace, mineral processing, and armour applications [1]. UD Ceramic Matrix Composites are mostly used in high temperature blast proof applications like face sheets for blast proof sandwich panels. These kind of high temperature composites are either manufactured by Hot Isostatic Pressing (HIP) or Powder Metallurgy, i.e., Compaction followed by Plasma arc sintering. Finding the homogeneous properties of the composite experimentally is an expensive process as these high temperature materials and its corresponding manufacturing process are expensive. So theoretical and numerical methods are employed to determine
the homogenous properties (i.e.) Young’s Modulus, Poisson Ratio and Shear Modulus of these materials. These properties are essential to carry out numerical modelling of these materials. Micromechanics is the most efficient tool to find the homogenous properties of the composite analytically and numerically [2]. Most of the available analytical and numerical models do not incorporate combined effects of matrix defects, interface defects and high temperature effects in a single model. Sadik L. Omairey [3] has developed a Python code, integrated with ABAQUS which calculates the effective properties of the unidirectional composite. ABAQUS is a popular finite element tool used for modelling highly non-linear problems with high accuracy [4]. These CMCs are basically used at very high temperature regimes like blast. So, estimation of these homogenous properties at elevated temperature. Hashin [5] has performed thermo-elastic analysis on composites at elevated temperatures. Eric W. Neuman et al [6] have experimentally determined the mechanical properties of ZrB2 at ambient and elevated temperatures. Modelling the interface defect is generally done by cohesive surfaces. Wu-Gui Jiang et al [7] have modelled and extracted the homogenous properties of the composite with imperfect interface. Y. Benveniste [8] uses cohesive surfaces at a variation of angle along the fiber-matrix interface to model the interface defects. Matrix and Fiber crack are mostly modelled using user subroutines.

Our goal is to homogenize the effective properties of the composites with all the above mentioned criteria. As our intention is to observe the trend in degradation of properties due to defects in the matrix and the interface, we have simplified the matrix crack into a ‘V’ notch with varying a/w ratios and 90° de-bonding between the fiber-matrix interface. For these mentioned cases, the homogenous properties were extracted and the degradation in properties is noted.

2. Finite Element Procedure

2.1 Modelling Representative Volume Element

The Representative Volume Element is modelled with unit dimensions with fiber embedded in the matrix. The fibre is unidirectional in nature and runs along the x axis of the geometry of RVE is shown in the figure 1.

![Figure 1. RVE of the Composite with Matrix and Fiber](image)

For modelling the RVE, commercial finite element solver ABAQUS is used. The assumptions considered prior to the modelling are that the fibers are placed in equal distances and the radius is same throughout the composite. It is also ensured that volume fraction criterion is satisfied.
2.2 Materials

The materials used for the homogenization are UD Fiber Reinforced Metal Matrix Composite and a UD Fiber Reinforced Ceramic Matrix composite. The UD CMC used in the study is Ultra High Temperature Ceramic Composite used for blast proof applications. The material properties of the matrix and reinforcements are listed in Table 1 and 2 as given below.

| Matrix         | E (GPa) | Nu (POISSON RATIO) |
|----------------|---------|--------------------|
| AA2024         | 73.1    | 0.33               |
| ZrB$_2$        | 500     | 0.11               |

Table 1. Matrix Properties of CMC and MMC.

Table 2. Fiber Properties of CMC and MMC.

| Reinforcement | E (GPa) | Nu   | G (GPa) |
|---------------|---------|------|---------|
| Silicon Carbide | $E_1$=403.2 | $\nu_{12}$=0.148 | $G_{12}$=93.1 |
|               | $E_2$=262.6 | $\nu_{13}$=0.148 | $G_{13}$=93.1 |
|               | $E_3$=262.6 | $\nu_{23}$=0.194 | $G_{23}$=109.5 |
| Alumina       | 373     | 0.27 |         |

In the case of matrix material, both MMC and CMC are considered to be isotropic in nature. However, the reinforcement Nextel 610 alumina fibre is considered as isotropic and Silicon Carbide fibre is considered as transversely isotropic. It is to be noted that after homogenization, the end result is a transversely isotropic material.

2.3 Periodic Boundary Condition

When it comes to homogenization of UD fiber reinforced composites, Periodic Boundary Conditions would fetch us exact results. Materials like fiber reinforced composites are generally represented as a repeated array of structures which is periodic. Periodic Boundary Condition implies that each RVE has same deformation and there is no separation between the neighbouring RVE’s. For a cubical RVE the displacement on the pair of opposite surfaces are given by equations 1 and 2.

\[ u_{i,j^+} = \varepsilon_{ik} x_{kj^+} + u_{i}^* \]  
\[ u_{i,j^-} = \varepsilon_{ik} x_{kj^-} + u_{i}^* \]  

where $j^+$ is along positive X direction and $j^-$ is along negative X direction. The difference of equations 1 and 2 is equation 3.

\[ u_{i,j^+} - u_{i,j^-} = \varepsilon_{ik} \Delta x_{kj} \]  

For an RVE, $\Delta x$ is a constant. So, the above equation reduces to equation 4.

\[ u_{i,j^+}(x,y,z)- u_{i,j^-}(x,y,z)=C_{ij}(i,j = 1, 2, 3) \]  

The constants, $c^{11}, c^{22}$ and $c^{33}$ represent the tensile or compressive behaviour on the RVE model due to the reaction of three normal traction components, whereas the other three pairs of constants, $c^{21} = c^{12}, c^{31} = c^{13}$ and $c^{32} = c^{23}$ correspond to the shear deformations due to three shear traction
components. This form of boundary conditions satisfies displacement periodicity. It can be seen from the above equation that the difference of the displacements for the corresponding points for a pair of opposite boundary surfaces are specified, but the individual displacement components are still functions of the coordinates.

The PBC is applied as a set of three boundary conditions for variation in the value of C:

**SET 1:** $C_1^1 = C_2^2 = C_3^3 = 0.012$ mm

**SET 2:** $C_1^1 = C_2^2 = 0.018$ mm

**SET 3:** $C_2^1 = C_3^1 = 0.016$ mm

**SET 4:** $C_3^1 = C_1^2 = 0.016$ mm where $i$ represents phase and $j$ represents direction.

Figure 2.1-2.4 represents output for 4 sets of boundary conditions for Aluminium-alumina composite and 3.1-3.4 represents ZrB2-SiC Composite.

**Figure 2.1.** Set 1 Boundary Condition

**Figure 2.2.** Set 2 Boundary Condition

**Figure 2.3.** Set 3 Boundary Condition

**Figure 2.4.** Set 4 Boundary Condition

**Figure 2.** Aluminium-Alumina Composite Outputs
2.4 Prediction of Elastic Constants

\[ [\varepsilon] = [S][\sigma] \]  

where \([S]\) is the compliance matrix in equation (4),

\[
[S] = \begin{bmatrix}
S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\
S_{12} & S_{22} & S_{23} & 0 & 0 & 0 \\
S_{13} & S_{23} & S_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & S_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & S_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & S_{66}
\end{bmatrix}
\]  

From the above matrix (5) the engineering elastic constants can be determined by following relations

\[
E_1 = \frac{1}{S_{11}} \quad N_{u12} = \frac{S_{12}}{S_{11}} \quad G_{12} = \frac{1}{2S_{44}}
\]

\[
E_2 = \frac{1}{S_{22}} \quad N_{u13} = \frac{S_{13}}{S_{11}} \quad G_{13} = \frac{1}{2S_{55}}
\]

\[
E_3 = \frac{1}{S_{33}} \quad N_{u23} = \frac{S_{23}}{S_{22}} \quad G_{23} = \frac{1}{2S_{66}}
\]
2.5 Results from Healthy Case Simulations

After applying the above described periodic boundary conditions and calculating the compliance matrix constants, the Young’s modulus, Poisson Ratio and Shear Modulus of the MMC and CMC with varying volume fraction from 20-47% is as shown in Figure 4.1-4.6 below. The corresponding figures below represent the variation of properties with respect to different debonding angles. Figures 4.1-4.6 represents variation of $E_1$, $E_2$, $\nu_{12}$, $\nu_{23}$, $G_{12}$, $G_{23}$ vs volume fraction.

![Figure 4.1. Vf vs E1](image1)

![Figure 4.2. Vf vs E2](image2)

![Figure 4.3. Vf vs G12](image3)

![Figure 4.4. Vf vs G23](image4)

![Figure 4.5. Vf vs Nu12](image5)

![Figure 4.6. Vf vs Nu23](image6)

**Figure 4:** Homogenous properties versus volume fraction

2.6 Inference from Healthy Case Simulation

With the outputs from Figure 4.1-4.6, the following inferences are made for variation of properties with respect to change in fibre volume fraction:

- As the MMC is Aluminium-Alumina, the properties are dominated by the fiber, the Young’s modulus along the fibre direction (i.e.) $E_1$ increases with increases by 46% at 47% fibre volume fraction.
• But the CMC is ZrB2-SiC where the matrix property completely dominates the fiber properties. So $E_1$ reduces by 5% as fibre volume fraction increases
• $E_2$ of the MMC increases by 53% and for CMC it reduces by 15%
• As both composites are transversely isotropic in nature $E_2$ and $E_3$ are same
• $G_{12}$ of MMC increases by 49% and decreases by 21% for CMC
• $G_{23}$ increases by 36% for MMC and reduces by 20% for CMC
• There is a decrease in Poisson’s Ratio as fibre volume fraction goes high for Aluminium-Alumina MMC, but for ZrB2-SiC CMC it almost remains a constant

3. Matrix crack:
The damage scenario in composite materials is peculiar when compared to metals. Failure in metals is defined by slow propagation of cracks, i.e., crack initiation and propagation in a series of notch blunting, while the failure in composites is a continuous process of damage growth, including various complicated failure mechanisms and damage modes. As our interest is in homogenizing the effective properties in the presence of defects in the matrix, crack initiation and propagation are not modelled. Instead, a ‘V’ notch with varying a/w ratios is modelled and the homogenization is performed. The ‘V’ notch model is given in the Figure 5.

![Figure 5. Composite with v notch](image)

The a/w ratio is varied from 0.02 mm to 0.1mm, and for all corresponding ‘V’ notches the effective properties are homogenized. Table 1 and Table 2 display the properties of the matrix and fibre materials. The corresponding figures below represent the variation of properties with respect to different a/w ratio. Figures 6.1-6.6 represents variation of $E_1$, $E_2$, $Nu_{12}$, $Nu_{23}$, $G_{12}$, $G_{23}$ vs a/w ratio

![Figure 6.1. a/w ratio vs $E_1$](image)

![Figure 6.2. a/w ratio vs $E_2$](image)
3.1 Inference from Matrix Defect

For 35% Fibre Volume fraction, for the variation of a/w ratio for 0.02-0.1 from the figure 6.1-6.6, following observations are made

- Matrix Crack doesn’t affect $E_1$ for both MMC and CMC, as the reduction is only 1% along the fibre direction.
- It doesn’t affect Poisson ratio’s of both the materials as they almost remain constant for variation of a/w ratios
- $E_2$ for ZrB2-SiC composite reduces by 2% for variation in a/w ratio and for Aluminium-Alumina Composite it reduces by 10%
- $G_{12}$ for ZrB2-SiC Composite reduces by just 1% and for Aluminium-Alumina composite it reduces by 5%
- $G_{23}$ for CMC reduces by 4% and for MMC it reduces by 2%
- $N_{12}$ and $N_{23}$ remain almost a constant for the CMCs but increases by 4% and 7% for MMCs

4. Interfacial Debonding:

Interfacial debonding is one major contributor for degradation of property of the composite. UD MMC and CMC are manufactured by either Hot Isostatic Pressing (HIP) of Powder Metallurgy (Compaction followed by Plasma Sintering). The issue occurs with debonding when the applied pressure in HIP process or Compaction process is not an optimum value. Debonding occurs when the applied pressure exceeds the optimum pressure value. Debonding generally degrades the transverse
tensile strength of the composite and it doesn’t affect the strength of the composite in the fibre direction. Experimental studies have revealed that the interfacial properties play a very significant role in affecting the effective orthotropic properties of the composite. Such imperfect interface in composite materials may arise from the presence of impurities at phase boundaries or sometimes due to wettability issues. These impurities are due to formation of oxide films or bonding agents at fibre/matrix interface. The existence of these imperfect interfaces will affect the overall effective property of the composite material significantly and thus leading to debonding of the fiber from the matrix and ultimately failure of the material.

4.1 Modelling Debonding

A 3D RVE is modelled with imperfect interface to study the effect of degradation of properties of the composite. The imperfect interfaces between the fiber and the matrix are taken into account by introducing cohesive contact surfaces. The influences of the interface on the elastic constants and the tensile strengths are examined through these interface models. The effect of the variation of the imperfect interface for every 90° of the fiber and matrix surface is studied. For every 90° the reduced cohesive stiffness is calculated and is assigned to the surface and the rest of the surface is tied to the matrix surface. The cohesive stiffness is calculated using given formula below

\[ K_{\text{interface}} = \frac{E_{\text{interface}}}{H_{\text{interface}}} \]

\[ E_{\text{interface}} = \frac{(E_{\text{matrix}} + E_{\text{fibre}})}{2} \]

\[ H_{\text{interface}} = 0.1 \times \text{Fiber radius, fibre radius} = 0.3338 \text{mm} \]

For Aluminium-Alumina Composite \( E_{\text{matrix}} = 73.1 \text{GPa} \) and \( E_{\text{fibre}} = 373 \text{GPa} \). For ZrB2-SiC CMC \( E_{\text{matrix}} = 500 \text{GPa} \) and \( E_{\text{fibre}} = 403.2 \text{GPa} \). \( K_{\text{interface}} \) for Zirconium – Silicon Carbide Composite is \( 1.3562 \times 10^7 \) and \( K_{\text{interface}} \) for Aluminium-Alumina Composite is \( 6.6982 \times 10^6 \). These corresponding stiffness values are assigned at every 90° variation in angle and the rest of the surface are tied. The rest of the homogenization procedure and the boundary conditions remain the same.

4.2 Output from corresponding boundary conditions:

The respective 4 sets of boundary conditions are applied on the RVE with induced defects and corresponding outputs for respective boundary conditions are shown in the figures given below. Figure 7.1-7.4 represents output with respect to 4 set of boundary condition for 0°-90° debonding. Figure 8.1-8.4 represents output with respect to 4 set of boundary condition for 0°-180° debonding. Figure 9.1-9.4 represents output with respect to 4 set of boundary condition for 0°-270° debonding. Figure 10.1-10.4 represents output with respect to 4 set of boundary condition for 0°-360° debonding.

![Figure 7.1. Set 1 BC](image1)

![Figure 7.2. Set 2 BC](image2)
Figure 7.3. Set 3 BC

Figure 7.4. Set 4 BC

Figure 7. Output for 0°-90° Debonding

Figure 8.1. Set 1 BC

Figure 8.2. Set 2 BC

Figure 8.3. Set 3 BC

Figure 8.4. Set 4 BC

Figure 8. Output for 0°-180° Debonding
Figure 9.1. Set 1 BC

Figure 9.2. Set 2 BC

Figure 9.3. Set 3 BC

Figure 9.4. Set 4 BC

Figure 9. Output for 0°-270° Debonding

Figure 10.1. Set 1 BC

Figure 10.2. Set 2 BC
4.3 Results:
The corresponding figures below represent the variation of properties with respect to different debonding angles. Figures 11.1-11.6 represents variation of $E_1$, $E_2$, $\nu_{12}$, $\nu_{23}$, $G_{12}$, $G_{23}$ vs debonding angle

**Figure 11.1.** Debonding angle vs $E_1$

**Figure 11.2.** Debonding angle vs $E_2$

**Figure 11.3.** Debonding angle vs $\nu_{12}$

**Figure 11.4.** Debonding angle vs $\nu_{23}$
4.4 Inference from Debonding Results:
For 35% Fibre Volume fraction, for the variation of debonding angle from ratio from 90°-360° following observations are made from figure 11.1-11.6

- Debonding doesn’t affect $E_1$ for both MMC and CMC
- Poisson ratio’s of both material remains a constant for variation of debonding angle
- $E_2$ for ZrB2-SiC Composite reduces by 46% from 0°-360° variation in debonding angle and for Aluminium-Alumina Composite it drastically reduces by 70%.
- $G_{12}$ for ZrB2-SiC Composite reduces by 37% and for Aluminium-Alumina composite it almost doubles about 71% reduction in $G_{12}$
- $G_{23}$ for CMC reduces by 45% and for MMC it reduces by 51%.

5. Conclusion:
The following conclusions were drawn from the above analysis between healthy case and the damage induced case

- $E_1$ for MMC increases by 46% from 20%-47% Fibre Volume fraction.
- Analysis for the crack and Debonding has been conducted for 35% Volume fraction where $E_1$ almost remains same for both matrix crack and debonding, as these phenomena doesn’t affect young’s modulus along the fibre direction.
- $E_1$ decreases by 5% as Fibre volume fraction increases for a CMC.
- The reason behind the reduction in $E_1$ is Young’s Modulus of the Matrix dominates young’s modulus of the fibre
- Transverse Young’s Modulus $E_2$ increases by 53% for MMC and reduces by 15% for the CMC
- With matrix crack the degradation of $E_2$ is only 2% for the CMC and 10% for the MMC
- Debonding degrades $E_2$ for both MMC and CMC in a large scale by 46% for CMC and 70% for MMC
- Poisson Ratio almost remains the same for all 3 cases for both CMC and MMC
- $G_{12}$ increases by 49% in MMC and decreases by 21% in CMC. Matrix crack only has very less effect of the degradation on CMC by 1% and % in MMC
- Debonding has a very high impact on $G_{12}$ reducing by 37% for CMC and has a very drastic effect on MMC by degrading it by 71%. $G_{23}$ goes down by 45% for CMC and 51% for MMC.

The above study shows that defects in the matrix doesn’t affect the properties much. On the other hand defects in the fibre matrix interface degrades the material to a larger scale by reducing its properties.
6. References

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