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Micro-Mechanical Analysis of Thermal Expansion of Damaged Composites

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Abstract: Micro mechanical theoretical and FE models have been developed to predict the Coefficient of Thermal Expansion (CTE) of unidirectional composites. The effects of matrix micro cracks and fiber/matrix interface debonding on CTE of composites were considered in the models. These two damages are assumed to affect CTE of composite via causing matrix stiffness degradation and introducing additional strain in interface debonding region, respectively. The model was adopted to predict the CTEs of glass fiber/resin matrix unidirectional composites with various fiber volume fractions and damage intensities. Meso FE models were built to validate the theoretical ones. The results reveal that the matrix damage could reduce CTE of unidirectional composites in longitude, however promote CTE in transverse. Fiber/matrix interface debonding could also bring notable increment of transverse CTE.

Key words: Unidirectional composite, micro-mechanics, micro-cracks, interface debonding, thermal expansion coefficient, CTE

INTRODUCTION

Composite structures might experience changes of temperature and humidity in large ranges during their operation life. For example, the environmental temperature GFRP (Glass Fiber Reinforced Plastic) made wind turbine blades exposed could cycle from -30°C to 50°C in a year. For the aircraft, more and more composite made components have been adopted and they experience even more rigorous work condition. The hypersonic vehicle thermal load acting on its quartz/ceramic composite made nose may >1000°C, the components of engines made by carbon/ceramic composites will bear temperature as high as 1200°C withal with high temperature gradient. The thermal expansion rate of composites which is one of the key performance indicators relates to the dimensional stability and thermal residual stress in structure and material. The micro-scale thermal mismatch stress between fiber and matrix in composites is one of the prime damage triggering and thereby affects the ultimate strength noticeably. Therefore, well understanding about the CTE (Coefficient of Thermal Expansion) and residual stress of composites is desirable for the purpose of predicting the mechanical properties of composite materials and composite structures.

Considerable research in this field have been found in literatures, e.g., He *et al*. (2002) developed meso mechanical theoretical and FE models of Si_3N_4/BN composite based on the authentic microscopic structure of material and the models were used in CTE prediction for unidirectional composite and orthogonal layered laminate. Agbossou and Pastor (1997) built a multi-parcel fiber model based on the energy equivalence to predict CTE and thermal mismatch stress of laminated materials. Moreover, the model could be used to analyze the impact of the interfaces between plies on thermal properties. Wu and Chen (2007) and Zhen *et al*. (2010) studied the thermo elastic properties of laminates using higher order local-global model in which compatibility of the transverse displacement between each layers along the thickness direction was considered. Karadeniz and Kumlutas (2007) set up a microscopic FE unit cell model to predict the CTE of unidirectional composites with various materials system and fiber volume fractions. They used their FE model to estimate the theoretical CTE models, they suggested and found in literatures. Karami and Garnich (2005) researched the influence of the fiber bending towards CTE of unidirectional composites using 3D microscopic FE model. Tan *et al*. (1999) developed numerical and theoretical models to predict average stiffness and CTE of 3D through the thickness angle interlock woven composites. Yilmaz and Dunand (2004) calculated the thermal mismatch stress in Cu-ZrW208 particle reinforced composites by 3D microscopic FE model and their research certified that thermal mismatch stress could cause phase changes sufficiently. Ohnuki and Tomota (1996) researched the anisotropy of CTE for whisker reinforced composites and validated their

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theoretical models by test data. Sideridis *et al.* (2005) built a 3-phase spherical model and obtained CTE of particle reinforced composites. Micro -matrix crack and fiber/matrix interface debonding are the susceptible damage in composites during the manufacturing and employing and they could affect material's CTE. Islam *et al.* (2001) established the micro scale FE model of unidirectional composite considering interface cracking and analyzed the impact of interface cracking on the CTE of different composite systems. Lu and Hutchinson (1995) investigated the influence of matrix cracks and interface debonding in brittle matrix unidirectional composites on CTE in longitude. In their model, the interface debonding sliding friction factor was considered. Fellah *et al.* (2007) analyzed the influence of plies with transverse cracking on CTE of laminates by an improved shear lag model. In this research, firstly micro mechanical theoretical CTE models of unidirectional composites including defects of micro-matrix cracks and fiber/matrix interface debonding have been developed. Then micro FE models were built to verify the theoretical ones. The CTEs of a glass fiber/resin matrix composite without defect and with various intensities of damages were predicted by these models.

MATERIALS AND METHODS

The thermal expansion model of composites considering matrix and interface damage: The CTEs of fiber and matrix in composites are usually not the same, e.g., CTE of polymer matrix might be one order higher than that of glass or carbon fiber. The overall thermal expansion rate of a composite depends not only on CTEs of fiber and matrix but also on the stiffness ratio of them. Micro-cracks in matrix reduce the average modulus of matrix and would affect the CTE of overall composite. If the micro-cracks distribute randomly, their affections on the average stiffness of matrix is isotropic. A fictive block of matrix material with volume of V contains number of M micro cracks and the average length of micro-cracks is denoted as $\bar{a}$. The density of micro-crack is defined as:

$$\gamma = \frac{M}{V}\bar{a}^3 \tag{1}$$

The elastic modulus of damaged matrix material, denoted as $\tilde{E}$ can be expressed as function of γ as (Shen, 1995):

$$\tilde{E}_m = E_m\left[1 - \frac{48}{45}\frac{(1-\tilde{\upsilon}^2)(2-\tilde{\upsilon})}{2-\tilde{\upsilon}}\gamma\right] \tag{2}$$

Here, E_m is the elastic modulus of virgin matrix, $\tilde{\upsilon}$ is Poisson's ratio of damaged matrix and it can be obtained from follow equation (Shen, 1995):

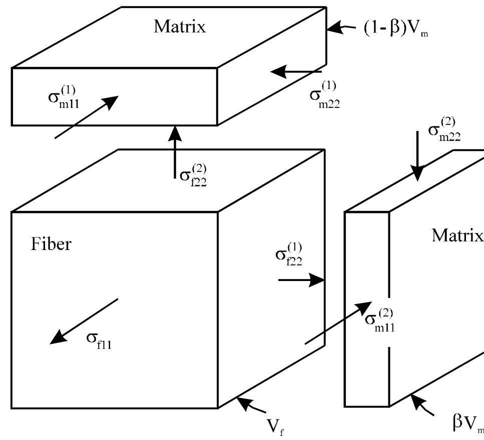

Fig. 1: Theoretical thermal expansion model of unidirectional composites

$$\gamma = \frac{45}{16}\frac{(\upsilon-\tilde{\upsilon})(2-\tilde{\upsilon})}{(1-\tilde{\upsilon}^2)\left[10\upsilon-\tilde{\upsilon}(1+3\tilde{\upsilon})\right]} \tag{3}$$

υ in Eq. 3 is the Poisson's ratio of undamaged material. As well known, the transverse properties of unidirectional composite both for stiffness and thermal/humid expansion are usually not precise enough calculated by simple lamellae model. In Lamellae model, transverse expansions combination of fiber and matrix are in series way so, the constraint between the deformations of the 2-phases has been lowly estimated. In this study, a modified model was suggested in order to sufficiently consider the restraint. In the new model as shown in Fig. 1, the cross section of fiber is simplified as square and matrix phase around fiber is classified to two parts. Part one (volume is $(1-\beta)V_m$) is supposed having identical mismatch stress (iso-stress) with fiber phase and part two (volume is βV_m) possessing the same mismatch strain (iso-strain) with fiber phase under thermal load. They are simplified as two slabs cement perfectly to fiber phase. Here, β is the volume proportion of the iso-strain part in matrix material. Under thermal load, the thermal mismatch stresses in part of fiber and two matrixes should be in equilibrium as follows:

$$V_f\sigma_{f11} - (1-\beta)V_m\sigma^{(1)}_{m11} - \beta V_m\sigma^{(2)}_{m11} = 0 \tag{4}$$

$$V_f\sigma^{(1)}_{f22} - (1-\beta)V_m\sigma^{(1)}_{m22} = 0 \tag{5}$$

$$V_f\sigma^{(2)}_{f22} - \beta V_m\sigma^{(2)}_{m22} = 0 \tag{6}$$

Here, V_f and V_m are the volume of the fiber and matrix, respectively. σ_{fii}, $\sigma_{mii}^{(k)}$ are the mismatch stresses in fiber phase and matrix phase, respectively, subscript i = 1, 2 denotes the direction parallel and perpendicular to the fiber direction, superscript k = 1, 2 refers the matrix parts their stress are iso-stress and iso-strain with the fiber along transverse direction, respectively. The deformation compatibility condition between fiber and matrix in the latitude and transverse directions are:

$$\alpha_{f11}\Delta T + \frac{\sigma_{f11}}{E_{f11}} - \frac{\upsilon_{f12}\sigma_{f22}^{(1)}}{E_{f11}} - \frac{\upsilon_{f12}\sigma_{f22}^{(2)}}{E_{f11}} = \alpha_m\Delta T - \frac{\sigma_{m11}^{(1)}}{\tilde{E}_m} + \frac{\upsilon_m\sigma_{m22}^{(1)}}{\tilde{E}_m} = \alpha_m\Delta T - \frac{\sigma_{m11}^{(2)}}{\tilde{E}_m} + \frac{\upsilon_m\sigma_{m22}^{(2)}}{\tilde{E}_m} \quad (7)$$

$$\alpha_{f22}\Delta T - \frac{\upsilon_{f21}\sigma_{f11}}{E_{f11}} + \frac{\sigma_{f22}^{(1)}}{E_{f22}} = \alpha_m\Delta T + \frac{\upsilon_m\sigma_{m11}^{(1)}}{\tilde{E}_m} - \frac{\sigma_{m22}^{(1)}}{\tilde{E}_m} \quad (8)$$

$$\alpha_{f22}\Delta T - \frac{\upsilon_{f21}\sigma_{f11}}{E_{f11}} + \frac{\sigma_{f22}^{(2)}}{E_{f22}} = \alpha_m\Delta T + \frac{\upsilon_m\sigma_{m11}^{(2)}}{\tilde{E}_m} - \frac{\sigma_{m22}^{(2)}}{\tilde{E}_m} \quad (9)$$

Where, α_{f11}, α_{f22} and α_m are the CTEs of fiber in axial direction, fiber in transverse direction and matrix, respectively, E_{fii} is the elastic modulus of fiber. Using the Eq. 4-9, we can find the thermal mismatch stresses in fiber and matrix then we can get axial and transverse CTEs of unidirectional composite. They are:

$$\alpha_{11} = \alpha_{f11} + \frac{\sigma_{f11}}{E_{f11}} - \frac{\upsilon_{f21}\sigma_{f22}^{(1)}}{E_{f22}} - \frac{\upsilon_{f21}\sigma_{f22}^{(2)}}{E_{f22}} \quad (10)$$

$$\alpha_{22} = \left(V_f + \beta V_m\right)\left(\alpha_{f22} + \frac{\sigma_{f22}^{(2)}}{E_{f22}} - \frac{\upsilon_{f21}\sigma_{f11}}{E_{f11}} - \frac{\upsilon_{f23}\sigma_{f22}^{(1)}}{E_{f22}}\right) + \left(1-\beta\right)V_m\left(\alpha_m + \frac{\upsilon_m\sigma_{m11}^{(1)}}{\tilde{E}_m} + \frac{\upsilon_m\sigma_{m22}^{(1)}}{\tilde{E}_m}\right) \quad (11)$$

When fiber/matrix interface debonds completely and temperature rise and CTE of matrix is larger than that of fiber, there will be no restraint between matrix and fiber. In this scenario, CTE of composite would be equivalent to that of the pure matrix. If volumetric ratio of interface failed fiber is V_{db} (and only complete interface debonding is considered), the transverse CTE of composites would be:

$$\alpha_{22}^{d\inf} = (1 - V_{db})\alpha_{22} + V_{db}\alpha_m \quad (12)$$

When interface debonds partly in annular instead of debonding completely, the restrain from fiber to the thermal deformation of matrix would decrease compared to the perfect interface case. The additive thermal expansion of the composite due to the partly interface damage is supposed direct proportional to the area ratio of damaged interface (denoted by $\gamma_{\inf}$); the discrepancy of CTEs between pure matrix material and the composite: α_m-α_{22}; the volume fraction of matrix in composites: 1-V_f. With these assumptions, the transverse CTE of partly interface damaged unidirectional composite is:

$$\alpha_{22}^{d\inf} = \alpha_{22} + \left(1 - V_f\right)\left(\alpha_m - \alpha_{22}\right)\gamma_{\inf} \quad (13)$$

In which $\gamma_{\inf}$ is defined as:

$$\gamma_{\inf} = \frac{1}{2\pi}\varphi \quad (14)$$

Where, φ is the radian of interface cracks relative to the fiber center. In this study, the effect from micro-matrix cracks on matrix CTE has been neglected. However, the matrix damage will reduce its average stiffness and in this way affect the CTE of composite. If the CTE of matrix is greater than that of fiber when temperature decreases matrix is tensioned in fiber direction and the transverse micro-cracks will open. Conversely when temperature increases matrix phase is compressed and transverse crack will be closed. Thermal expansion of whole composite will be affected by the opening/closure of micro-cracks. This thermal unilateral condition has not been included in this study and it is being studied in the subsequent researches.

The micro scale Finite Element Analysis (FEA) of composites' CTE: To validate the theoretical thermal expansion model suggested in previous chapter, a micro scale FE model was built to investigate CTE and local thermal mismatch stresses in composites. In unidirectional composites fibers usually distribute randomly and composites can be considered as transverse isotropic materials. Here, fibers are supposed packing in hexagonal pattern. As shown in Fig. 2, a periodic rectangular section

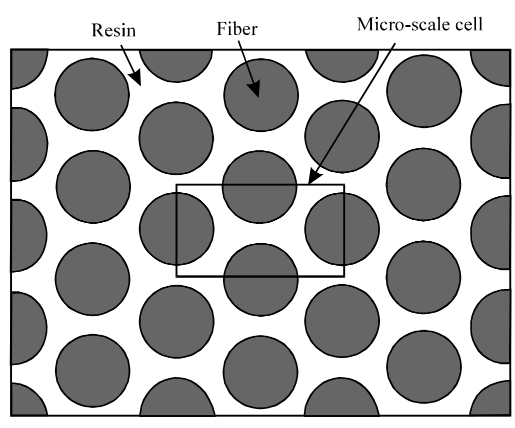

Fig. 2: Micro-scale unit cell

framed by black lines is adopted as the micro scale cell for unidirectional composites. The unidirectional composites can be imaged assembled with a great number of micro scale unit cells and the physical properties obtained from one unit cell could represent the average level of the whole composite. To satisfy the displacement continuum condition in other words, there would be no overlapping and disengagement between adjoined cells, the periodic boundary conditions should be applied to the unit cell model. Xia *et al*. (2003) offered a general periodic boundary condition expression suitable for implementation in FEM.

Figure 3 is a schematic graph to demonstrate the way to apply the periodic boundary condition to the micro-scale unit cell. The micro-scale unit cell is cut from the inside of the fiber bundle, therefore it is periodical along the three directions of space. If its three coordinate planes are chosen as the master planes, nodes on them are master nodes, the three other planes opposite to them are chosen as their corresponding slave planes. The three corner points B-D are set as master nodes. The displacements in slave planes, denoted as $u_i^{b'}$, $u_i^{c'}$ and $u_i^{d'}$ are the combinations of the displacements of their master nodes in master planes denoted as u_i^b, u_i^c and u_i^d and master corner points denoted as u_i^B, $u^C{}_i$ and $u^D{}_i$ as following:

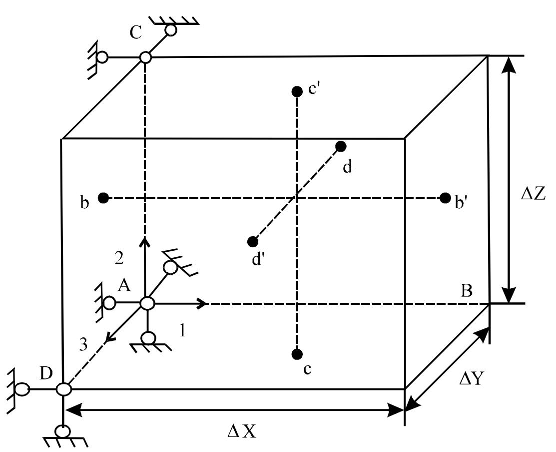

Fig. 3: Periodic boundary conditions of micro-scale cell

$$u_i^{b'} = u_i^b + u_i^B, \quad u_i^{c'} = u_i^c + u_i^C, \quad u_i^{d'} = u_i^d + u_i^D \quad (i = 1, 2, 3) \tag{15}$$

CTE of the unit cell can be expressed as:

$$\alpha_{11} = (u_i^{d'} - u_i^d)/\Delta Y \Delta T, \quad \alpha_{22} = (u_i^{b'} - u_i^b)/\Delta X \Delta T \tag{16}$$

Here, ΔT is temperature increment and ΔX, ΔY are the side lengths of unit cell as shown in Fig. 3.

Numerical example and analysis: A fictitious glass fiber/resin matrix unidirectional composite is adopted for verifying damage included thermal expansion model. The elastic constants and CTE of fiber and matrix are shown in Table 1.

Here, researchers assume β = 0.435 (Eq. 4) and the CTEs of undamaged composites with various fiber volume fractions predicted by theoretical model (Eq. 4-11) and FE model are both shown in Table 2.

From Table 2, there find that both longitude and transverse CTEs predicted by theoretical model in this study have less discrepancy with FEM results compared to those calculated by existing model with fiber volume fraction ranges from 35-80%.

In micro-scale FE model, micro-cracks are simulated by opening nodes of adjoined elements. The micro-matrix and interface cracks are both pictured with black bold lines in Fig. 4a, b, respectively. When temperature increases, matrix will be compressed in fiber direction, therefore the transverse micro-matrix cracks (or the transverse component of micro-matrix cracks) will close. For simplification in FE model, the micro-matrix cracks are modeled without transverse projection component, i.e., the normal directions of micro-crack surfaces

Table 1: Parameters of glass fiber and resin

Parameters	E/GPa	υ	α (10^{-6}/°C)
Glass fiber	73.0	0.2	5
resin	3.5	0.4	40

Table 2: CTE of composites with various fiber volume fractions (10^{-6}/°C)

Vf /%	35	40	45	50	55	60	65	70	75	80
Study of Shen and Kai (2006)	7.96	7.43	7.01	6.66	6.37	6.12	6.91	5.73	5.57	5.43
α_{11}										
This study	8.76	8.07	7.43	6.97	6.60	6.30	6.04	5.82	5.64	5.48
FEM	8.25	7.72	7.25	6.87	6.51	6.30	6.14	5.92	5.70	5.55
α_{22}										
Study of Shen and Kai (2006)	35.87	33.62	31.33	29.00	26.65	24.29	21.90	19.51	17.11	14.70
This study	34.04	31.66	29.29	26.93	24.30	22.30	20.02	17.78	15.57	13.39
FEM	34.01	31.70	29.33	27.02	24.71	22.40	20.15	17.96	15.84	13.45

perpendicular to the fiber direction. In the cross section plane of unidirectional composites, the micro-matrix cracks could be viewed distributing in two dimensional. Their density could be rewritten as:

$$\gamma_m = \frac{M}{S}\bar{a}^2 \tag{17}$$

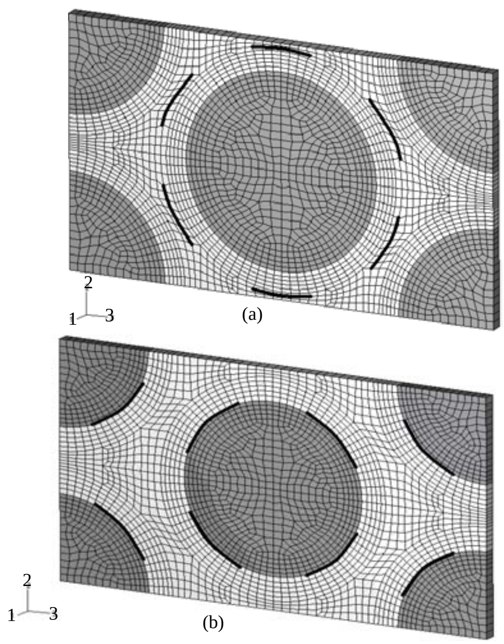

Fig. 4: Micro-scale FE model with damage; a) micro-matrix cracks and b) Fiber/matrix interface debonding

Here, S is the area of 2-3 plane of unit cell in Fig. 4. In FE model, the interface damage is also defined by Eq. 14. The damage effects brought by micro-matrix cracks on axial and transverse CTEs of unidirectional composite are shown in Table 3 and 4, respectively. Compared with Table 3 and 4, we find that due to the matrix damage, CTE of composites reduces in fiber direction while increases in transverse. In fiber direction, the overall thermal expansion of composite is the sum of free thermal deformation of fiber and the elastic deformation caused by thermal mismatch stresses (Eq. 10). When matrix damaged, the later would diminish due to the decline of mismatch stresses. From Eq. 11, there can also find that the diminishing matrix modulus and mismatch stresses might increase the dominate terms which related with these two factors. Table 3 and 4 also demonstrate that CTEs predicted by theoretical model and FE model, respectively are in well agreement. Transverse CTE of interface damaged composites is showed in Table 5. From Table 5, there can find that the impact of interface damage is trivial on the fiber directional CTE but significant on transverse CTE. When interface damage occurs, transverse CTE of composite increases obviously. This is because fiber interface debonding weakens the fiber constraint effect on matrix thermal expansion. Figure 5a-c show distributions of local stresses, local strain and micro cracks opening on the micro-scale cell with matrix damage when temperature increases 100°C (with fiber volume fraction of 55%). From Fig. 5a, it is observed that when temperature increases matrix is compressed while

Table 3: Axial CTE of unidirectional composite with matrix damage (10^{-6}/°C)

Vf /%	35	40	45	50	55	60	65	70	75	80
γ = 0.1										
FEM	8.20	7.75	7.21	6.86	6.55	6.28	6.07	5.87	5.68	5.50
This study	8.43	7.75	7.22	6.81	6.47	6.19	5.96	5.76	5.59	5.44
γ = 0.3										
FEM	7.65	7.14	6.72	6.40	6.14	5.88	5.71	5.53	5.36	5.25
This study	7.68	7.15	6.74	6.42	6.15	5.94	5.75	5.60	5.46	5.35

Table 4: Transverse CTE of unidirectional composite with matrix damage (10^{-6}/°C)

Vf /%	35	40	45	50	55	60	65	70	75	80
γ = 0.1										
FEM	34.83	32.57	30.01	27.70	25.31	23.03	20.77	18.58	16.51	14.11
This study	34.12	31.75	29.38	27.03	24.70	22.39	20.12	17.87	15.65	13.46
γ = 0.3										
FEM	35.10	32.93	30.68	28.50	26.32	24.13	22.01	19.95	17.94	15.71
This study	34.31	31.95	29.59	27.25	24.93	22.62	20.34	18.08	15.84	13.63

Table 5: Transverse CTE of unidirectional composite with various fiber volume fractions and interface debonding damage degrees (10^{-6}/°C)

Vf /%	35	40	45	50	55	60	65	70	75	80
γ = 0.25										
FEM	35.10	32.76	30.36	28.02	25.68	23.35	21.07	18.85	16.73	14.28
This study	35.01	32.91	30.76	28.57	26.33	24.07	21.77	19.45	17.09	14.72
γ = 0.5										
FEM	37.30	34.95	32.54	30.21	27.77	25.42	23.75	20.86	18.73	16.27
This strudy	35.98	34.16	32.23	30.20	28.07	25.84	23.52	21.11	18.62	16.05

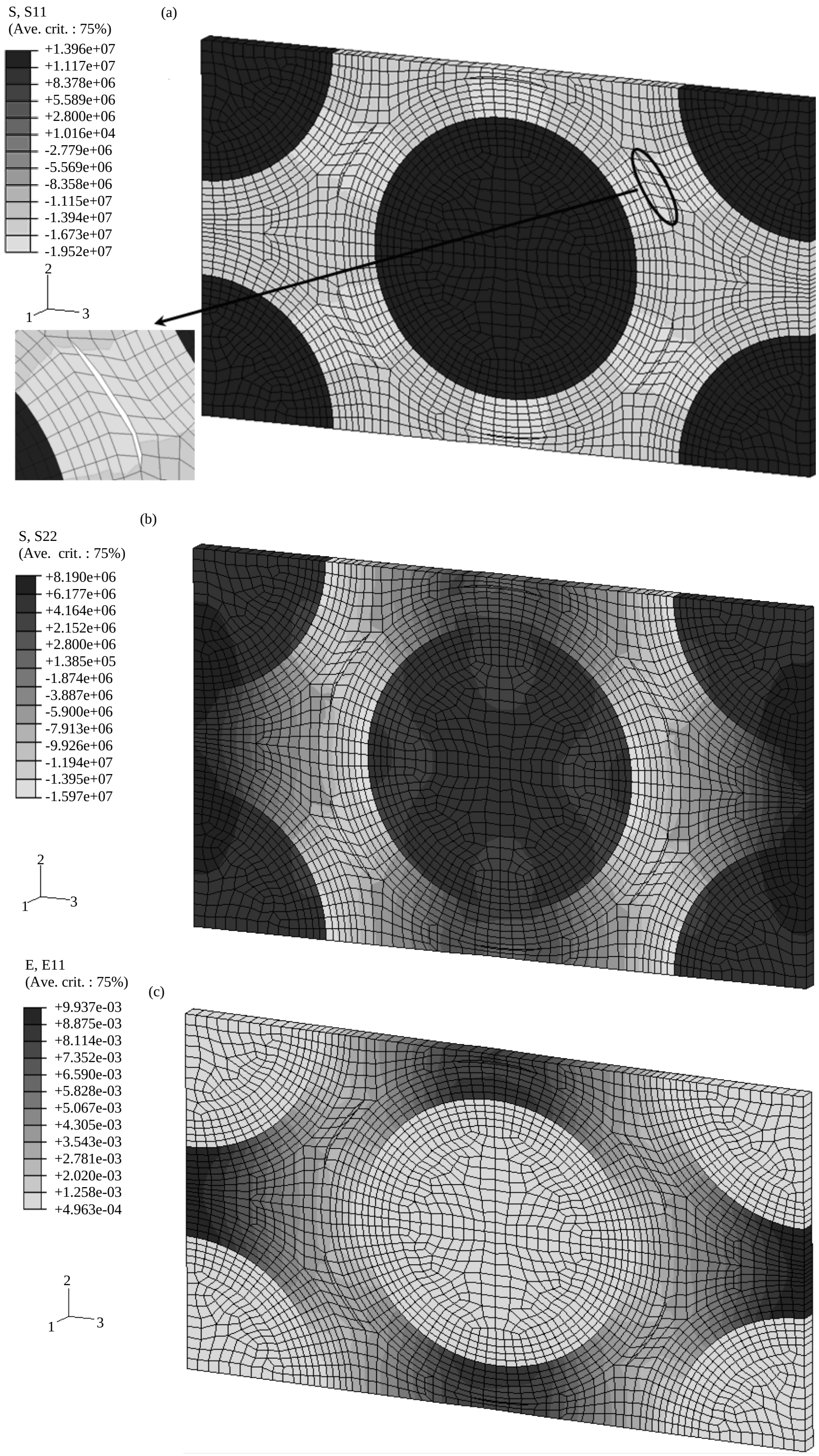

Fig. 5: Continued

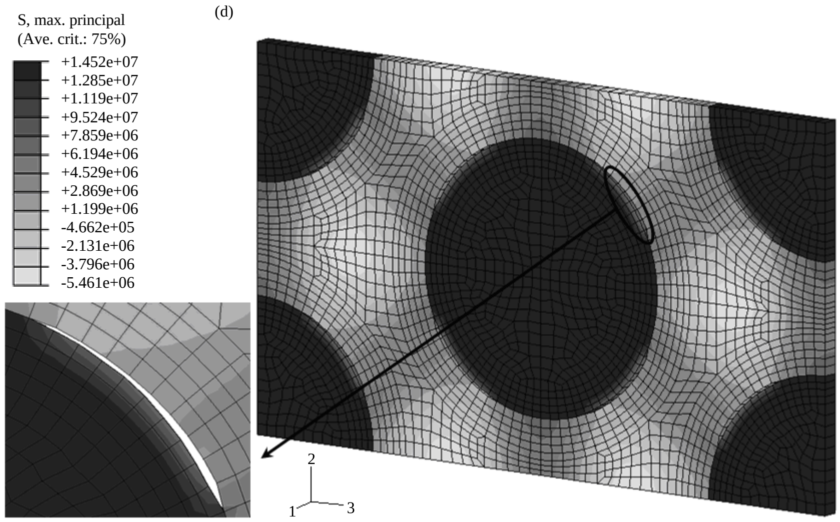

Fig. 5: Deformation and distribution of local stress and strainwith damage (V_f = 55%); a) local stress σ_{11} with matrix damage of γ_m = 0.1; b) local stress σ_{22} with matrix damage of γ_m = 0.1; c) local strain ε_{22} with matrix damage of γ_m = 0.1 and d) local maximum principal stress with interface cracks of γ_{int} = 0.5

fiber is tensioned in the fiber direction. One can also find that in some region (left and right lateral region of unit cell), the transverse normal stress, e.g., σ_{22} are continues in fiber and matrix (Fig. 5b) while transverse strain, e.g., E_{22} increases abruptly from fiber to matrix (Fig. 5c). This part could be considered as iso-stress region. Contrarily in some other region (left and right lateral region of the central fiber), the discrepancy of transverse stresses (σ_{22}) between fiber and matrix is notable (Fig. 5b) while the transverse strains are continuous there (Fig. 5c). Thus, this area is approximately iso-strain region. Figure 5a-c show the reasonability of the theoretical model developed in this study.

Local stress and micro-crack opening of the fiber interface damaged composite (the material parameters and temperature load are the same with Fig. 5a-c) is shown in Fig. 5d. It also shows that during the expansion, the three pairs of opposite surfaces still keep parallel and the continuities of both displacement and stress are satisfied.

CONCLUSION

In this study, the effects of micro-matrix cracks and fiber/matrix interface debonding on CTE of unidirectional composites were investigated theoretically. Micro FE models were built to validate the theoretical ones. The results reveal that the existence of matrix damage would reduce CTE of composites in longitude but advance in transverse. The fiber/matrix interface damage could advance the transverse CTE of composites, however has trivial impact on CTE in longitude. And the predicted CTE by theoretical model and FE model are in well agreement.

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