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Development of an Elastic Functionally Graded Interphase Model for the Micromechanics Response of Composites

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Abstract—A new micromechanics framework is developed for long fibre reinforced composites using a single fibre surrounded by a functionally graded interphase and matrix as a representative unit cell. The unit cell is formulated to represent any number of aligned fibres by a single fibre. Using this model the elastic response of long fibre composites is predicted in all directions. The model is calibrated to experimental results and shows very good agreement in the elastic regime. The differences between the proposed model and existing models are discussed.

Keywords—Computational mechanics, functionally graded interphase, long fibre composites, micromechanics.

I. Introduction

In order to expand the use of composite materials within the automotive industry, predictive material models are required to facilitate product development. Researchers are interested in the use of composite materials for use in automotive structure for energy absorption [1], [2]. The largest issues with current composite material models is that none are able to predict all composite failure modes [3]. Failure in long fibre reinforced composite materials can be broken down into three generalized categories: fibre failure, matrix failure and interface failure. To predict these three generalized failure modes a material needs to be based on a micro scale approach to separate the material responses of the fibre matrix and interface between the two.

Aboudi's method of cells is one of the most prevalent composite micromechanics models, where two isotropic materials are combined in a repeating unit cell to predict the overall response of the composite material [4]. Recently the use of cohesive elements to predict the onset of interface failure between the fibre and matrix, which are modeled separately [5], [6]. These models are computationally expensive as they use contact algorithms and many elements to model a single fibre.

A new framework to model composite materials based off a micromechanics approach has been developed by Sabiston et al. [7]. The model uses a functionally graded interphase surrounding a representative fibre to capture the stress transfer between the fibre and matrix. The model is compared to experimental results from Kyriakides et al. and Hsiao and Daniel [8], [9].

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II. Methodology

A three dimensional unit cell model is developed containing a single representative fibre. This unit cell is used to account for the material response of composites through implementation in a finite element software. A model is developed where the properties of the fibre and matrix are used to calculate the stress in each constituent, then combined to find the overall response of the material.

A. Unit Cell Development

Ideally the unit cell should be representative regardless of the physical quantity of fibres within the domain of the unit cell. Considering the cross section of a region of interest containing fibres, the volume fraction of fibres within that area is equivalent to the cross sectional area of the fibres. Assuming that the fibres are round the cross sectional area of a fibre is

$$A_f = \pi r_f^2. \tag{1}$$

With the region of interest being one unit in area, the number of fibres within the region is given by

$$n_f = \frac{V_f}{A_f}. \tag{2}$$

It is assumed that the fibre radius (r_f) is constant.

Using an interface to represent the force transfer between the fibre and matrix is a very common approach. In our arbitrary unit cell the quantity of interface is equivalent to the surface area of the fibres which is equivalent to the circumference of the fibre multiplied by the length. Given that the unit cell has one unit of volume and dimensions on one unit in each direction, the surface area of a fibre is its circumference. Therefore, multiplying the surface area of the fibres by the number of fibres in the unit cell and simplifying, the area of interface in the unit cell is

$$A_i = \frac{2V_f}{r_f}. \tag{3}$$

The quantity of interface is dependent on the radius of the fibres in the composite. Therefore, the fibres need to be

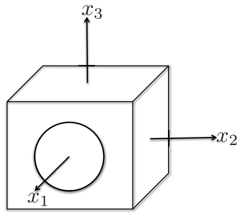

Fig. 1 Unit Cell Configuration

included at a one to one scale to correctly account for the interaction between the fibre and matrix.

Another approach to account for the interaction between the fibre and matrix is to assume that an interphase surrounds the fibre. The interphase has it's own material properties and occupies a volume surrounding the fibre. It is assumed that the outer boundary on this interphase is proportional to the fibre radius. Using a proportionality constant p multiplied by the fibre radius to define the boundary of the interphase, the volume of interphase surrounding one fibre is

$$V_{int} = (p-1)r_f^2. \tag{4}$$

Multiplying (4) by the number of fibres yields the volume of interphase within the unit cell which is given by

$$V_i = \frac{(p-1)V_f}{\pi}. \tag{5}$$

In the case of an interphase the quantity of interphase is only a function of the volume fraction and not the fibre radius. Therefore through the use of an interphase a single representative fibre is capable of representing any number of actual fibres, and a region of interest can be modeled as only having one fibre.

The unit cell model contains a single fibre aligned with the x_1 direction of the unit cell. The faces of the unit cell are located at one unit in each direction. A diagram of the unit cell is given in Fig. 1.

The radius of the representative fibre in unit cell coordinates is

$$r_{rf} = \sqrt{\frac{4V_f}{\pi}}. \tag{6}$$

The interphase zone starts inside the fibre and continues outside the fibre. The start and finish radii of the interphase zone are proportional to the representative fibre radius and are given by (7) and (8) respectively.

$$r_{is} = kr_{rf} \qquad 0 < k < 1 \tag{7}$$

$$r_{if} = lr_{rf} \qquad l \geq 1 \tag{8}$$

The material paring parameters k and l are assumed to be constant for a given material pairing and are dependent on the fibre and matrix in the composite.

B. Unit Cell Mechanics

The material properties of the interphase zone need to be established. To obey material compatibility and equilibrium there needs to be continuity between the stresses for a given strain. This works if the moduli are identical between the fibre and matrix; however, this is not generally the case in composite materials where the advantage of the material comes from having a large differential in stiffness between the fibre and matrix.

To maintain equilibrium for a given strain it was devised that the material modulus within the interphase must change as a function of position. This function is described in terms of cylindrical coordinates around the x_1 axis of the unit cell. The value of the two end points of the functions are known (r_{is}, E_m) and (r_{if}, E_f).

Using the two end points functions describing the variation of modulus within the interphase zone are defined, which are known as interphase functions. They are used to calculate the overall response of the unit cell through the use of the known elastic constants of the fibre and matrix. This is done by integrating the interphase functions to find a representative radius where the properties transition between that of the fibre and matrix.

C. Interphase Functions

Using the two end points a linear and two quadratic functions were derived to describe the transition of Young's modulus between the fibre and matrix as presented in [7]. Using the two end points as values of a function, a linear interphase function follows logically where the modulus is described as a function of radius within the bounds of the interphase function given in (9).

$$E(r) = \frac{1}{r_{if} - r_{is}}\left[(E_m - E_f)r + E_f r_{if} - E_m r_{is}\right] \tag{9}$$

For a quadratic equation there needs to be three points to fully define the function. As only the values at the end points of the function are known a third point is defined by setting the derivative of the function to zero at one of the end points. In general this is done by taking the derivative of a general quadratic equation in the form

$$ax^2 + bx + c = 0, \tag{10}$$

which has a derivative of the form

$$\frac{a}{2}x + b = 0. \tag{11}$$

By setting the derivative to zero at one of the end points the function is fully described. The first function describing the radius as a function of elastic modulus within the interphase zone has its derivative evaluated at (r_{is}, E_f). This function is given in (12) [7].

$$r(E) = \frac{r_{if} - r_{is}}{(E_m - E_f)^2}(E - E_f)^2 + r_{is} \tag{12}$$

The second quadratic interphase function has a derivative evaluated at the end point (r_{if}, E_m), where modulus is described as a function of radius given in (13) [7].

$$E(r) = \frac{E_f - E_m}{(r_{if} - r_{is})^2}(r - r_{if})^2 + E_m \tag{13}$$

A graph showing a comparison of the three interphase functions is shown in Fig. 2. The boundaries on the interphase zone were arbitrarily set at $r_{is} = 0.5$ and $r_{if} = 0.8$, with a fibre modulus of 217 GPa and a matrix modulus of 3.5 GPa.

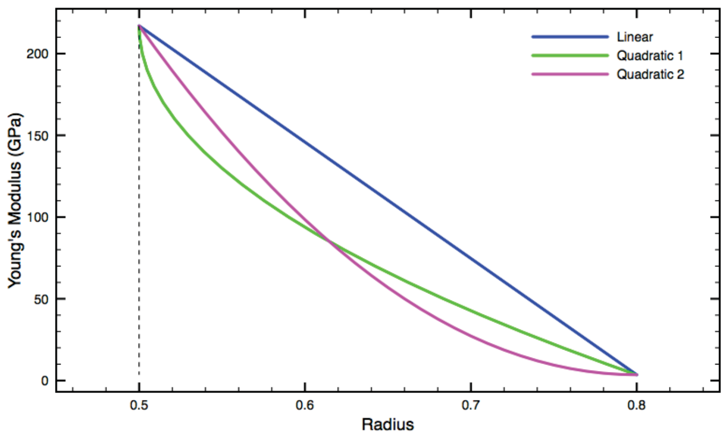

Fig. 2 Comparison of the three interphase functions in the interphase zone

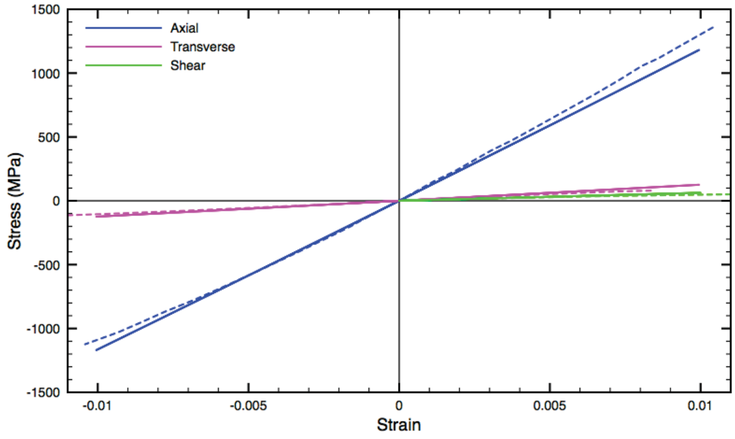

Fig. 3 Comparison between proposed model and Kyriakides et al. [8]

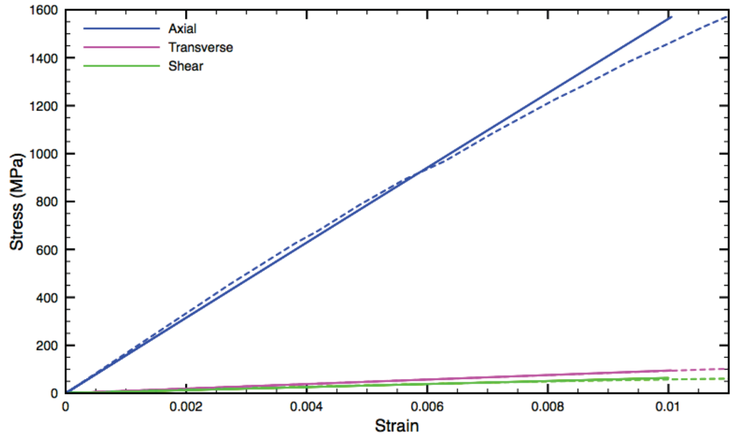

Fig. 4 Comparison between proposed model and Hsiao and Daniel [9]

D. Interface radii

The interphase functions are integrated in circular cylindrical coordinates within the interphase zone to find a volume which is equated to the volume of a tube with an outer radius equivalent to a step transition between the modulus in the fibre and that of the matrix. The tube has the same inner bounds as the interphase zone start radius r_{is} and the outer radius is called the representative interface radius r_{ri}. This radius is given in terms of difference in Young's modulus and the interphase parameters in (14).

$$r_{ri} = \sqrt{\frac{V_{\Delta E}}{\pi(E_f - E_m)} + r_{is}^2} \tag{14}$$

The difference in Young's modulus is found through the general integral

$$V_{\Delta E} = \int_0^{2\pi} \int_{r_{is}}^{r_{if}} \int_{E_m}^{E(r)} r dE dr d\theta, \tag{15}$$

with the exception of the first quadratic interphase function (12) where the integration is done in the order

$$V_{\Delta E} = \int_0^{2\pi} \int_{E_m}^{E_f} \int_{r_{is}}^{r(E)} r dr dE d\theta. \tag{16}$$

Using the combination of (14) and (15) or (16) and the interphase functions the representative interface radii are calculated. For the linear interphase function (9) the interface radius is

$$r_{ri} = \sqrt{\frac{1}{3}\left(r_{if}^2 + r_{if} r_{is} + r_{is}^2\right)}. \tag{17}$$

For the first quadratic interphase function (12) the interface radius is

$$r_{ri} = \sqrt{\frac{1}{5} r_{if}^2 + \frac{4}{15} r_{if} r_{is} + \frac{8}{15} r_{is}^2}. \tag{18}$$

For the second quadratic interphase function (13) the interface radius is

$$r_{ri} = \sqrt{\frac{1}{6} r_{if}^2 + \frac{1}{3} r_{if} r_{is} + \frac{1}{2} r_{is}^2}. \tag{19}$$

These three representative interface radii are then used to combine the constitutive equations for the fibre and matrix to predict the overall response of the composite system.

E. Material Models

The stress in each constituent is calculated using the elastic constitutive law for the fibre or matrix L_f and L_m respectively. The matrix is assumed to be isotropic elastic with two elastic constants and the fibre is assumed to be transversely isotropic with five elastic constants. The strain in each material is assumed to be the same. The stresses are combined through volumetric averaging to find the overall stress. The volume of material which acts like the fibre is found using the representative interface radius.

$$V_{rf} = \frac{\pi}{4} r_{ri}^2 \tag{20}$$

The stress from each constituent are combined to calculate the overall stress in the unit cell as

$$\sigma = (1 - V_{rf})\sigma_m + V_{rf}\sigma_f, \tag{21}$$

where σ_m and σ_f are the stresses in the matrix and the fibre respectively. The overall stress can also be calculated from the strain and combining the constitutive laws as

$$\sigma = [(1 - V_{rf})L_m + V_{rf} L_f]\varepsilon \tag{22}$$

TABLE I
MATERIAL PROPERTIES AND CALIBRATION DATA

Parameter	Kyriakides et al. [8]	Hsiao and Daniel [9]
Fibre Axial Modulus (GPa)	214	279
Fibre Transverse Modulus (GPa)	13.8	13.8
Fibre Transverse Poisson's Ratio	0.2	0.3
Fibre Transverse Axial Poisson's Ratio	0.28	0.3
Fibre Shear Modulus (GPa)	13.8	13.8
Matrix Modulus (GPa)	4.10	2.31
Matrix Poisson's Ratio	0.356	0.35
Interphase Function	Quadratic 2	Quadratic 2
Interphase Parameter k	0.71	0.70
Interphase Parameter l	1.0	1.0

F. Implementation

The model was implemented into the explicit dynamic finite element code LS-DYNA through a user defined material model. The inputs to the model are: the interphase function either linear or one of the quadratic functions along with parameters k and l. Seven material parameters are input for the elastic properties of the fibre and matrix. A displacement control boundary condition is used to deform one element to replicate experimental results.

III. RESULTS AND DISCUSSION

Experimental results from Kyriakides et al. [8] and Hsiao and Daniel [9] where used for comparison with the proposed model. The material properties used for the calibration of the model are given in Table I, where the material properties not given from the papers were found from the work of Chamis [10]. Both of these sets of experimental data were selected for having stress strain results in multiple directions allowing a proper calibration and validation of the proposed model.

The simulation results for the data from Kyriakides is given in Fig. 3 where the experimental results are given by dashed lines and the simulation results in the solid lines.

As is demonstrated the simulation matches very closely to the experimental data for the elastic region of the stress strain curve. The simulation is only run to 1% strain as above these strain levels there is separation in the stress strain response due to plasticity in the matrix material and the onset of failure.

The simulation results compared to the data from Hsiao and Daniel is shown in Fig. 4 where as with the previous the experimental results are shown in the dashed line and the simulation results are in the solid line.

As with the results from Kyriakides the model shows very good predictive capabilities for predicting the axial, transverse and shear stress strain response of the composite. There are deviations from linear in the experimental results at strains nearing 1% this is especially true in the axial direction. These results are for compression and as a result there is likely fibre micro buckling occurring under axial compression.

In the current implementation it is assumed that the strain is equal in the fibre and the matrix. This has been shown to be a decent approximation from the results as there are not large disparities in the transverse behaviour of the model. This can be attributed to the use of the transversely isotropic fibre material model, which allows for a reduced modulus in the transverse direction. In general it is known that due to the difference in modulus between the fibre and matrix there must be some accommodation of strain where the amount of strain in the fibre and matrix is different. This behaviour has been described by Eshelby for an inclusion within isotropic materials [11].

As the average stress in the fibre and matrix can be separated from this model it allows for the implementation of a stress based failure criterion for the fibre and matrix separately. This offers an improvement over existing theories which account for failure through the generalized stress state such as the theory proposed by Hashin [12]. The separation of the stress strain response for strains above 1% needs to be accounted for in future work. A model for the matrix accounting for plasticity is required to improve these predictive capabilities for larger strains. The addition of failure into the model will also contribute to the predictive capabilities.

IV. Conclusion

A new frame work is developed using a functionally graded interphase to account for the micromechanics interaction of a fibre and matrix. The model allows a single fibre to be representative of any number of aligned fibres in a composite material. This model is capable of separating the stress in the fibre and matrix allowing for implementation of failure models based on the stress in the constituents. This model offers the advantage of simplicity and efficiency over existing models.

The proposed model is capable of accurately predicting the elastic stress strain response of composite materials using established elastic constants for the material and two interphase parameters k and l. This model provides a framework to develop a complete three dimensional composite failure model as demonstrated through its elastic capability.

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