MICROSCOPIC MODELING OF TOW MECHANICAL BEHAVIOR IN WOVEN FABRIC FORMING

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ABSTRACT

A micromechanical modelling is derived for a bundle of carbon filaments in a tow with polymer material coated on the exterior surface in sizing process. The model predicts the evolution of the microstructure and filament characteristics on the mechanical properties of tow in compressive loading. A regular pattern is assumed for the distribution of filaments in the microstructure of a carbon fiber tow. The mechanical response of tow is examined on the compressive loading condition considering large deformation and rearrangement of filaments in the microstructure as well as the contact properties between filaments and filaments with the polymeric coating. The micromechanical modelling obtains new distribution of filaments in the microstructure, deformation of polymeric coating, the compressive loading-displacement curve and the maximum stress in polymeric coating which is used in the failure analysis. With this modelling effort, we aim to support the experimental findings in a qualitative manner. The proposed model provides a physically sound understanding of mechanical properties of tows and in the development of the corresponding constitutive law at large deformation of woven fabric in forming process.

1 INTRODUCTION

Forming dry fabric is the initial step in production of woven-fabric reinforced composites using the resin transfer molding process. The production of defect free parts in a reasonable cost requires a fundamental knowledge and systematical understanding of textile deformation in manufacturing process. An exact model is required to analyze forming process and obtain details such as stress distribution in yarns, the reasons of yarn failure, formation of hole and fiber condensation areas due to movement of tows, effects of friction on the structural rearrangement, crimp interchange and onset of structure locking due to tow rotation [1]-[2]. Development of a simulation tool for fabric forming requires characterization of the mechanical properties of fabrics. The deformation of an individual tow influences the shape of cross-section, which in turn has an effect on the formability of stacked plies of woven fabric. The first stage for the deformation analysis of carbon woven fabric is to model individual tow which is a bundle of thousands of continuous individual carbon filaments held together and protected by an organic coating, as shown in Fig. 1. The frictional behavior of fibrous tows during processing typically involves intra-tow (on the microscopic filament scale), inter-tow, and tow–metal interactions [3]. To date, little work has been done to provide an approach to relate the material behavior on the filament scale (micro-scale) to that on the tow scale (meso-scale).

A carbon filament is a long, thin strand of cylinder with diameter of 5–10 micrometers and is classified by the tensile modulus including low, intermediate, high and ultrahigh modulus values. The carbon filament is produced from a polymer such as polyacrylonitrile (PAN), rayon, or petroleum pitch, known as a precursor. About 90% of the carbon fibers are made from polyacrylonitrile (PAN). The precursor is drawn into long strands or fibers and then heated to a very high temperature (1,000-3,000° C) for several minutes in a furnace filled with a gas mixture without oxygen to prevent burning. The high temperature causes the atoms in the fiber to vibrate violently until most of the non-carbon atoms are expelled. This process is called carbonization and leaves a fiber composed of long, tightly inter-locked chains of carbon atoms with only a few non-carbon atoms remaining. After carbonizing, the fibers have a surface that does not bond well with matrix materials used in composites. The filament surface is slightly oxidized by addition of oxygen atoms to provide better chemical bonding properties
and also etches and roughens the surface for better mechanical bonding properties. Oxidation can be achieved by immersing the fibers in various gases such as air, carbon dioxide, or ozone; or in various liquids such as sodium hypochlorite or nitric acid. The fibers can also be coated by electrolytic procedure in which the fibers are as the positive terminal in a bath filled with various electrically conductive materials. The sizing process is done by holding together a bundle of filaments and coating them with materials compatible to matrix materials such as epoxy, polyester, nylon, and urethane. The sizing process protects the filaments from damage during winding or weaving, reduces fuzz and increases the interfacial shear strength between the fibers. The weight of sizing materials is 0.5 to 5 percent of the weight of the carbon fiber. The coated fibers are wound onto cylindrical bobbins which are loaded into a spinning machine and the fibers are twisted into yarns of various sizes.

The modeling of woven fabrics can be studied in three different levels including macroscopic, mesoscopic and microscopic scales. Homogenized models can be derived in the macroscopic scale to represent the fabric as a plate or a shell. At a mesoscopic scale, the yarns or tows are considered as continuous media and the behavior of fabrics have been studied considering the fabric as an assembly of interlacing tows. The mechanical behavior of individual fibers has to be taken into account to describe the behavior of woven structures at a microscopic scale. There are only a few numerical models which regard composite fabric as composed of individual fibers at the microscale.

Durville simulated the behavior of samples of woven fabrics considering the individual fibers (nearly 500 fibers) with a particular attention on the detection and modeling of contact-friction interactions occurring within the collection of fibers. Wang and Sun established the concept of a digital-element, in which yarns were modeled by a pin-connected digital-rod-element chain. Dobrich et. al. modeled a unit cell of dry textiles using a numerical method in combination of digital element approach. The model was implemented in LS-DYNA to analyze the in-plane properties of dry textile. Due to the computational cost, the tows contain only a relatively few fibers, far from the situation of real fabrics with thousands of fibers in a tow.

The current research work presents a micromechanical modelling for a bundle of filaments in tows to predict the evolution of tow microstructure and filament characteristics on the mechanical properties at large deformation. A regular pattern is assumed for the distribution of a large number of filaments in the microstructure of the carbon fiber tow with polymeric coating. The mechanical response of tow is examined on the compressive loading condition considering large deformation and rearrangement of filaments in the microstructure as well as the contact properties between filaments and filaments with the polymeric coating. The micromechanical modelling obtains new filaments distribution in the microstructure, deformation of polymeric coating, the compressive loading-displacement curve and the maximum stress in polymeric coating which is used in the failure analysis.
2 MICROMECHANICAL MODEL

Consider a tow as a bundle of carbon filaments and the external surface of tow coated with nylon material in the sizing process. The filaments are come into contact because of tensile force applied to them during sizing process. Since the sizing process is performed in automated machine with exact control on fiber tensile force and placement, a regular pattern is considered for the fiber distribution in the tow cross section. It is assumed that the cross section of fibers is circle with the same diameter and pattern is identical along two orthogonal axes 2 and 3, as shown in Fig. 2. The adjacent fibers, which are in contact in the reference configuration, can separate, slip and push against each other during the deformation process.

![Figure 2: The idealized fiber distribution in the tow cross section](image)

The displacement of fibers in the cross section of tow causes that the internal force is generated between fibers. As shown in Fig. 3, the internal force can be divided into two groups as follows:

1. Contact force between two adjacent fibers
2. Axial force of polymeric coating due to relative displacement of two fibers connected by coating materials;

**Contact force:** Fig. 3a shows two adjacent filaments inside the tow. The filaments apply contact force to each other when the distance between two adjacent fibers is less than the diameter of filaments. The theory of contact between elastic bodies is used to relate the contact force and indentation depths for two cylinders with parallel axes. It was shown [13] that the force between two identical elastic cylinder is linearly proportional to the width of cylinders \( L \), the indentation depth \( \varphi \) and elastic modulus of fiber \( E_f \) and the corresponding Poisson ratio \( \nu_f \) as follows:

\[
f'_c = \begin{cases} \frac{\pi E_f L}{8(1-\nu_f^2)} \varphi & \varphi \leq 0 \\ 0 & \varphi > 0 \end{cases}
\]

where \( f'_c \) is the contact force along the line connecting fibers \( I \) and \( J \). The current position of fibers \( I \) and \( J \) is used to defined a unit vector \( \mathbf{t} = t_1 \mathbf{i} + t_2 \mathbf{j} \) along the connecting line. The current distance between two fibers is calculated based on the position vectors of the center of fibers, namely,

\[
s_{ij} = \sqrt{\sum_{i=1}^{2} (x_{ji} - x_{ii})^2}
\]

where \( x_{ji} \) and \( x_{ii} \) are the components of current position vectors for the center point of fibers \( I \) and \( J \), respectively. The indention depth is calculated as the difference of current distance between two fibers and the diameter. The internal force vector between two fibers can be written as:
Two types of internal forces applied to the fibers including a) Contact force between two adjacent fibers, b) Axial force of polymeric coating due to relative displacement of two fibers connected by coating materials.

\[
\begin{align*}
    f_{ij}^{\text{int}} &= -f_{ji}^{\text{int}} = f_i^t t = \begin{cases} 
    \frac{\pi E_f t L}{\delta (1 - \nu_f^2)} (s_{ij} - d) & (s_{ij} - d) \leq 0 \\
    0 & (s_{ij} - d) > 0 
    \end{cases} 
\end{align*}
\]  

**Axial force of polymeric coating:** Fig. 3b illustrates schematically the polymer layer coated on the exterior boundary of tow. The layer causes that two filaments located on the boundary cannot freely separate and the corresponding linear element has different stiffness values in compressive and tensile axial deformation. Assuming a hyper elastic model for resin material, the axial stress along linear element \( S_e \) is proportional to the positive Green strain for tensile deformation of linear element, namely \( S_e' = E_r \varepsilon_e' \), where \( E_r \) is the elastic modulus of polymeric coating and \( \varepsilon_e' \) is the Green strain along the rod axis which is expressed by

\[
\varepsilon_e' = \frac{s_i^2 - S_{ij}^2}{2S_{ij}^2} \quad (s_{ij} - d) > 0
\]  

where \( s_0 \) is the initial length of linear element. The current distance between tow fibers in the current configuration is given by

\[
S_{ij} = \sqrt{\sum_{i=1}^{2} (x_{ji} - x_{ki})^2}
\]

Based on the rectangular section of polymeric coating described by the fiber length and coating thickness \( h \), the internal force due to axial deformation of polymeric coating is expressed as:

\[
\begin{align*}
    f_{ji}^{\text{int}} &= -f_{ij}^{\text{int}} = E_r h L \frac{s_i^2 - S_{ij}^2}{2S_{ij}^2} t
\end{align*}
\]

3 **COMPUTATIONAL APPROACH**

The discrete model for the deformation of carbon filaments is a nonlinear and discontinuous problem.
Total time is divided into several time steps and the displacement and velocity vectors at the end of step time are calculated based on the corresponding vectors at the start of increment and, external force and boundary conditions. An implicit solution method is used to solve the governing equation to obtain the displacement vector as well as the force applied to the carbon filaments. The equation of motion of filaments at time steps is given by

\[ \mathbf{f}(t) = \mathbf{f}^{\text{ext}}(u(t), t) - \mathbf{f}^{\text{int}}(u(t), t) \]  

(7)

In the general form, the external and internal forces are dependent on the time as well as the current displacement and velocity vectors. The internal force of a filament is calculated based on the amount of gap functions between filaments and corresponding adjacent filaments and polymeric coating. Although the contact force between adjacent fibers limited the displacement of fibers moving towards each other along the line connecting between center of fibers, the distance between fibers can freely increase in the present discrete model for fibers inside the cross-section of tow. The implicit solution method may be singular for some internal fibers. Since the surface of carbon fibers is fuzz, the fibers cannot separate and some internal force should be considered between separating fibers. For simplicity, the stiffness of separating force is considered as one order of magnitude less than the stiffness of contact force.

The initial values for displacement vector are used to start the incremental analysis. Using Newton-Raphson solution method for the nonlinear problem, the displacement vector for the new increment is calculated based on the external and internal force vectors. The position vector of the center of fibers is updated for each iteration in a given increment and the iterative procedure is repeated until the residual force tends to zero value with a convenient accuracy. The procedure is repeated to calculate the deformation for each increment up to the final time instant.

4 RESULTS AND DISCUSSION

The cross section of carbon filaments is considered as circle with identical diameter 10μm, which are distributed in the cross section of an elliptical tow with major and minor axes of 1.6mm and 0.2mm, respectively [2]. The filament distribution pattern is assumed to be identical along the orthogonal axes 1 and 2, as shown in Fig. 2. The carbon filaments are elastic material with elastic modulus of 400 GPa and Poisson ratio 0.2. The polymeric coating of tow is made of nylon materials with elastic modulus of 3.0 GPa. The polymeric coating with thickness of 10μm connects the fibers on the external boundary of tow.

Fig. 4a illustrates the discretize model for filaments in the cross section of tow. A quarter of tow is considered for geometrical symmetry with respect to the planes \( x_1 = 0 \) and \( x_2 = 0 \). The component of displacement vector normal to symmetry planes is zero for the filaments located on the symmetry planes. In addition to, the internal filaments cannot pass the symmetry planes and the normal displacement is set to zero when they touch the symmetry planes. A rigid plane normal to \( x_2 \)-axis is moved with constant speed to compress the tow geometry. At the initial instance, the rigid plane touches the polymeric coating of the filaments located at the maximum \( x_2 \)-value. The vertical movement of rigid plane causes that more filaments are come into contact of rigid plane. The present model is used to calculate the displacement of filament and the deformed geometry of polymeric coating at any time instant. As shown in Fig. 4b, the movement of rigid plane causes that the contacting filaments have the same vertical velocity equal to the velocity of rigid plane. The displacement of such filaments is transfer to the internal filaments and the horizontal distance between internal filaments is increased in order to move filaments between the other filaments. The polymeric coating acts as a belt limiting the horizontal movement of filaments and holding the filaments into the cross section.

The present model is also used to calculate the force applied to the filaments and the polymeric coating of tow. The loading of the filaments inside the tow is calculated based on the contact force of adjacent filaments, while the filaments attached to polymeric coating may subject to the axial loading as well as the contact force of adjacent filaments. The filaments at the symmetry planes are subjected to both support loading and contact force. The internal force vectors are used to calculate the total compressive force required to deformed tow at different time increment, as shown in Fig. 5. At each time increment, the list of filaments contacting the rigid body is obtained. The compressive force is calculated as the sum of vertical component of internal force applied to the contacting filaments with...
the rigid surface. As the deformation proceeds, the stiffness of tow increases because of excessive contact points between fibers especially at the vertical centerline.

Figure 4: A quarter of the cross section of a single tow: a) the initial configuration, b) the deformed geometry after axial strain 4.3% along vertical axis

Figure 5: The calculated compressive force required to apply the transverse strain to tow

The results are used to determine the distribution of tangential axial stress of polymeric coating and predict the polymer rupture at the excessive deformation of tow. Fig. 6 shows the maximum value of tensile axial stress in polymeric coating at different compressive strain. The source of axial strain in
coating is the penetration of a filament inside the cross section between two filaments attached with polymeric coating. The tensile strain resulting in the rupture of coating layer can be determined based on the strength of polymeric coating and the maximum value for polymer tensile stress calculated by the micromechanical model.

Figure 6: The calculated maximum value for strain applied to the polymeric coating of tow

5 CONCLUSIONS

A micromechanical model is developed based on the discrete element method to characterize the compressive response of carbon tow. The micromechanical model estimates a nonlinear stiffness for tow in transverse loading. The discretize model can conveniently predict the movement of filaments inside the cross section. The theory of contact between elastic bodies describes the interaction between adjacent filaments inside the cross-section of tow. The polymeric coating, which connecting filaments at the exterior surface of tow, acts as a belt limiting the horizontal movement of the filaments and holding the filaments into the cross section. The hyperelastic model describes the mechanical behavior of coating material which is subjected to considerable axial stretch and rotation during compressive loading of tow. Such model can predict the rupture of polymeric coating at excessive deformation.

REFERENCES


