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Micromechanical modeling of the wood cell wall considering moisture absorption

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ABSTRACT

This paper constructs a micromechanical framework to study the modulus loss of the wood cell wall induced by moisture absorption. The wood cell wall is modeled as an infinite matrix containing circular cylindrical inhomogeneity. The matrix, composed of hemicellulose and lignin, can uptake large amounts of water and as a result cause remarkable modulus loss below fiber saturation point. Considering the swelling strain distributed in the matrix rather than in the inhomogeneity, two sub-problems are constructed. One is an equivalent eigenstrain problem where the eigenstrain is distributed in the inhomogeneity, and another is a uniform swelling strain distributed in both matrix and inhomogeneity. The modulus loss of the matrix is treated as a damage process that correlates with the moisture content. Based on the Mori-Tanaka method, the proposed micromechanical framework is employed to predict the effective stiffness of the wood cell wall under different moisture contents. Theoretical predictions of the tensile modulus under different microfibril angles (MFAs) and moisture contents agree well with available experimental results.

1. Introduction

The wood fiber has been used as reinforcement in various natural wood composites since they are environment-friendly and have high specific modulus and strength. Despite rather good knowledge about mechanical modeling of wood composites on macroscopic scale [1–5], little effort is devoted to theoretical analysis of the wood cell wall from a microscopic level. Existing researches on this topic mainly focus on experimental studies [6–8]. Therefore, a deep understanding of the wood cell wall structure is of great importance in modeling the wood cell wall.

There are three constituent materials in the wood cell wall: cellulose microfibril (CMF, 40–50 wt%), hemicellulose (25 wt%) and lignin (20–30 wt%) [9]. The CMFs as reinforcement with circular cylindrical shape are enclosed by a matrix composed of hemicellulose and lignin, so that they can be modeled as long fiber reinforced composites under the micromechanical framework based on inclusion method. Various micromechanical schemes have been successfully used in obtaining effective properties of composite materials [10–14]. Among them the Mori-Tanaka scheme [15,16] is employed in this paper because of its simplicity and without loss of generality.

The CMFs, with tensile modulus along longitudinal direction as high as 120–170 GPa, show little affinity to moisture absorption in its crystal region, and almost maintains its original mechanical properties in a humid environment above fiber saturation point (FSP) [8,17]. By contrast, the hemicellulose with elastic modulus as lower as 2 GPa, is strongly hydrophilic which has remarkable softening effects on its mechanical properties. Such softening phenomenon becomes more obvious after more water uptake. For instance, the elastic modulus of hemicellulose decreases even to 20 MPa when it is fully saturated [18].

Other than the moisture content, the microfibril angle (MFA) defined as the orientation of the specific microfibril with respect to the longitudinal cell axis, also plays an important role in mechanical properties of the wood cell wall [6]. The cell wall structure usually consists of several layers with different MFAs [19], among which the S_2 layer occupying 80–90% of the total volume of the wood cell wall, is the thickest and dominates its mechanical properties [20].

There are several computational analyses of the wood cell wall structure, for example, the finite element simulation of its extensibility [6] and the multi-scale numerical model of its creep behavior [21]. However, the moisture-dependent properties are

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rarely taken into consideration in the existing theoretical or computational analyses.

In fact, the analysis of moisture-dependent properties of the wood cell wall is very similar to that of natural fiber composites, in which the inhomogeneity is hydrophilic and the matrix is usually hydrophobic [22]. Pan and Zhong [16] proposed a micromechanical model to simulate the mechanical degradation of natural fiber composites by a modified Mori-Tanaka method with two damage variables. Through solving an equivalent eigenstrain problem, the overall deformation and mechanical properties of natural fiber composites are determined with the consideration of moisture absorption. However, for the wood cell wall, the difference is that the inhomogeneity is hydrophobic while the matrix is hydrophilic. Motivated by the successful application of the modified Mori-Tanaka model in natural fiber composites [16], the analysis of the wood cell wall is conducted through constructing and solving an equivalent eigenstrain problem.

The paper is organized as follows. A general micromechanical framework of the wood cell wall is constructed in Section 2, in which the modified Mori-Tanaka method [16] is employed to establish the basic equations of the wood cell wall. In Section 3, we particularize the proposed micromechanical model with unidirectional oriented inhomogeneities of circular cylindrical shape under. Then in Section 4, the predicted tensile moduli along the cell axis are compared with the available experimental results under different MFAs and moisture contents. Further discussions of the present micromechanical model are made in Section 4. Finally in Section 6, we draw the conclusions.

2. Micromechanical framework

The microstructure of the wood cell wall is shown in Fig. 1, which is composed of hemicellulose, lignin and cellulose microfibril (CMF) aligned along a given direction (x_3-axis). The microfibril angle (MFA) φ is defined as the angle between x_3-axis and the cell axis (x_3'-axis). The microstructure of the wood cell wall is analog to that of a long fiber reinforced composite [18], so that the CMFs can be treated as transversely isotropic inhomogeneities (denoted as Ω) of infinite length. The inhomogeneities are orientated unidirectionally and embedded in an infinite matrix (denoted as $D-\Omega$) that is composed of hemicellulose and lignin. The inhomogeneities are assumed to be hydrophobic and free of any initial strain and stress, while the matrix is strongly hydrophilic and subject to a swelling strain ε^s in a humid environment. The governing equations and boundary conditions for this problem are given, as follows:

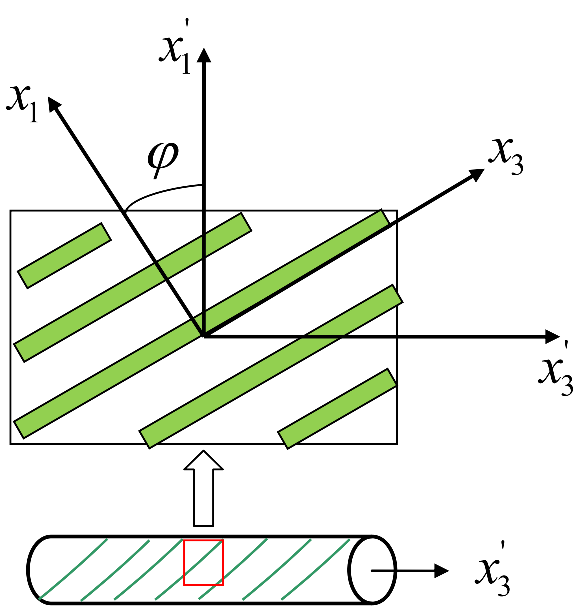

Fig. 1. An illustration of the wood cell wall structure and the plane problem under the global and the local coordinates.

$$\begin{cases} \nabla\cdot\boldsymbol{\sigma}^{(i)}=0 \quad \boldsymbol{\varepsilon}^{(i)}=\frac{1}{2}\left(\nabla\mathbf{u}^{(i)}+\mathbf{u}^{(i)}\nabla\right) & \text{in D} \\ \boldsymbol{\sigma}^{(1)}=\mathbf{C}^{(1)}:\boldsymbol{\varepsilon}^{(1)} & \text{in } \Omega \\ \boldsymbol{\sigma}^{(2)}=\mathbf{C}^{(2)}:\left(\boldsymbol{\varepsilon}^{(2)}-\boldsymbol{\varepsilon}^{s}\right) & \text{in D}-\Omega \\ \left[\boldsymbol{\sigma}^{(1)}-\boldsymbol{\sigma}^{(2)}\right]\cdot\mathbf{n}=0 \quad \text{and} \quad \mathbf{u}^{(1)}=\mathbf{u}^{(2)} & \text{on } \partial\Omega \\ \boldsymbol{\sigma}^{(2)}=0 & \mathbf{x}\to\infty \end{cases} \tag{1}$$

where, and throughout the paper, a boldface letter stands for a second or fourth-order tensor, a colon between two tensors denotes a contraction (inner product) over two indices, $\partial\Omega$ denotes the interface between Ω and $D-\Omega$, $\boldsymbol{\sigma}^{(i)}$, $\varepsilon^{(i)}$, $\mathbf{u}^{(i)}$ and $\mathbf{C}^{(i)}$ $(i=1,2)$ are respectively the stress, the strain, the displacement and the stiffness of the inhomogeneities (labeled by the superscript '1') and the matrix (labeled by the superscripts '2'). The notation $[\bullet]=(\text{out})-(\text{in})$, $\mathbf{n}$ is the outward unit normal on the interface, and $\nabla=\mathbf{i}_m\frac{\partial}{\partial x_m}$ is the Hamilton derivative operator with $\mathbf{i}_m$ being the unit direction vector. It is difficult to solve Eq. (1) directly by a classic eigenstrain problem, because the initial eigenstrain is distributed in the matrix, rather than in the inhomogeneity. Hence, the original problem given by Eq. (1) is further decomposed into two sub-problems as illustrated in Fig. 2, which can be solved by employing the Eshelby solution for the classic inclusion problem with a given eigenstrain.

In Sub-problem I, a swelling strain ε^s is uniformly distributed both in the inhomogeneities and the matrix, without any other external mechanical loads, so that the governing equations and boundary conditions for Sub-problem I can be written as

$$\begin{cases} \nabla\cdot\boldsymbol{\sigma}^{(i),\mathrm{I}}=0 \quad \boldsymbol{\varepsilon}^{(i),\mathrm{I}}=\frac{1}{2}\left(\nabla\mathbf{u}^{(i),\mathrm{I}}+\mathbf{u}^{(i),\mathrm{I}}\nabla\right) & \text{in D} \\ \boldsymbol{\sigma}^{(1),\mathrm{I}}=\mathbf{C}^{(1)}:\left(\boldsymbol{\varepsilon}^{(1),\mathrm{I}}-\boldsymbol{\varepsilon}^{s}\right) & \text{in } \Omega \\ \boldsymbol{\sigma}^{(2),\mathrm{I}}=\mathbf{C}^{(2)}:\left(\boldsymbol{\varepsilon}^{(2),\mathrm{I}}-\boldsymbol{\varepsilon}^{s}\right) & \text{in D}-\Omega \\ \left[\boldsymbol{\sigma}^{(1),\mathrm{I}}-\boldsymbol{\sigma}^{(2),\mathrm{I}}\right]\cdot\mathbf{n}=0 \quad \mathbf{u}^{(1),\mathrm{I}}=\mathbf{u}^{(2),\mathrm{I}} & \text{on } \partial\Omega \\ \boldsymbol{\sigma}^{(2),\mathrm{I}}=0 & \mathbf{x}\to\infty \end{cases} \tag{2}$$

Here the superscript 'I' denotes physical quantities for Sub-problem I.

As for Sub-problem II, an initial eigenstrain $-\varepsilon^s$ is imposed only in the inhomogeneities, and the matrix is free of any external mechanical loads and initial eigenstrains. Therefore, the governing equations and boundary conditions for Sub-problem II are given as

$$\begin{cases} \nabla\cdot\boldsymbol{\sigma}^{(i),\mathrm{II}}=0 \quad \boldsymbol{\varepsilon}^{(i),\mathrm{II}}=\frac{1}{2}\left(\nabla\mathbf{u}^{(i),\mathrm{II}}+\mathbf{u}^{(i),\mathrm{II}}\nabla\right) & \text{in D} \\ \boldsymbol{\sigma}^{(1),\mathrm{II}}=\mathbf{C}^{(1)}:\left[\boldsymbol{\varepsilon}^{(1),\mathrm{II}}-\left(-\boldsymbol{\varepsilon}^{s}\right)\right] & \text{in } \Omega \\ \boldsymbol{\sigma}^{(2),\mathrm{II}}=\mathbf{C}^{(2)}:\boldsymbol{\varepsilon}^{(2),\mathrm{II}} & \text{in D}-\Omega \\ \left[\boldsymbol{\sigma}^{(1),\mathrm{II}}-\boldsymbol{\sigma}^{(2),\mathrm{II}}\right]\cdot\mathbf{n}=0 \quad \mathbf{u}^{(1),\mathrm{II}}=\mathbf{u}^{(2),\mathrm{II}} & \text{on } \partial\Omega \\ \boldsymbol{\sigma}^{(2),\mathrm{II}}=0 & \mathbf{x}\to\infty \end{cases} \tag{3}$$